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Feasibility study: modelling environmental concentrations of chemicals from emission data

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Executive summary

The purpose of this feasibility study is to develop a toolbox of available methodologies and a work plan for applying relevant models to substances reported under the European Pollution Emission Register (EPER) in order to predict the composition and distribution of these chemicals in the European environment — in effect, the 'chemical density' of Europe. The study aims to identify which of the available chemical models are sufficiently validated and accepted to be used in a policy context and which models are suitable for substances listed under EPER. The focus of the study will therefore be specifically on models suitable for large industrial point source emissions, with emphasis on models suitable for manufactured chemicals and heavy metals.

The work, which has been undertaken in two phases, consists of the following tasks:

Phase 1

1. Identify available models.
2. Verify their status of validation and general acceptance.
3. Evaluate selected models for their ability to provide information on the spatial distribution of chemicals in the different environmental media in the geographical area of the EEA member country and participating states.
4. Scan models and provide information on the time and spatial scale they cover, provide expert judgement on the resolution needed for assessment of (pan) European, national, regional or local pollution and describe model characteristics for each level.
5. Identify which models are applicable to EPER substances.

Phase 2

6. Run one or more models for a test substance using EPER database releases to map chemical concentrations, identify 'hot spots' assess usefulness of EPER data for this purpose, and compare predicted concentrations with measured values, if available.
7. Draft a work plan to extend Task 6 to all relevant models identified in Task 5.
8. Develop a strategic proposal on how these models and derived data can be used to estimate the chemical density in the European environment based on emission data.
9. Summarise the findings in the final report.

The findings from Phase 1 of the study were reported in an interim report submitted in May 2005. This final report presents developments made under the completion of the study in Phase 2, building on the strategy from the interim report stage. A draft of this final report has been reviewed at an international summer school on chemical modelling held in Brno in July 2005 and at an expert workshop held in Copenhagen on 16 August 2005. This final report takes into account the feedback from the review of the draft report.

The principal **conclusions** of this feasibility study are as follows:

1. Predicting the chemical density of Europe from emissions data will require access to appropriate models and the data needed to drive them.
2. A large number of models are available for predicting environmental concentrations of chemicals in single or multiple environmental media. Many of these models are well-established in terms of history of usage in policy or regulatory applications, have been peer-reviewed and used as the basis of many peer-reviewed scientific papers. Most of these models are readily available, either for purchase or as freeware. Most will run on current Microsoft Windows® based personal computers commonly in general use and some may be run interactively over the Internet. A few require a more sophisticated platform, such as Unix or Linux workstations. Some established models, notably EMEP models, are not publicly available, at least at present.
3. Models range from highly complex spatially and temporally resolved models capable of predicting small scale variations in chemical concentrations in one or more environmental media, to simpler screening tools that predict concentrations averaged over wider spatial and temporal domains. A number of leading models have been identified for specific applications that are particularly well-established and which could form the basis of a set of tools for modelling chemical density from emissions data. The study has not attempted to identify the 'best' model for any particular purpose: this is outside the current remit and would

be a major Task in its own right. A number of inter-comparison studies have been completed, or are underway under the auspices of EMEP for several well-established multimedia models for regional/hemispherical modelling of POPs and mercury. These have not so far established clear benefits of one model over another.

4. A wide range of factors determines the fate of chemicals in the environment. These factors relate to the process of the release itself and how the substance is dispersed into the receiving medium; the properties of the chemical that determine its persistence and mobility (such as vapour pressure, partition coefficients, degradation rate constants in various media, etc.); meteorological and hydrological factors spatially and temporally disaggregated at the appropriate level that affect the dispersion of the substance and also landscape characteristics (also spatially and temporally disaggregated) such as vegetation type, coverage, land use, etc. Local scale air dispersion models, for example, need detailed information on the release characteristics and local topography and meteorology at the time of release: spatially-resolved multimedia models require a full set of input data relating to the factors listed above.
5. On the other hand, screening type models have much lower requirements for input data and usually characterise the receiving environment in terms of broad average landscape properties, meteorology and hydrology. A screening model, EUSES, has been endorsed by the European Commission for chemical risk assessment in compliance with the requirements of its official technical guidance. It is important to note that highly detailed models will not provide greater accuracy of output than a simpler screening model unless the input data is characterised with the required degree of certainty and that all relevant processes are simulated appropriately.
6. It is anticipated that a great deal of effort would be required to predict the chemical density of Europe through detailed modelling of all EPER releases. In addition to the highly resource-intensive work needed to run detailed models and to assess and interpret the results correctly, a more important constraint is the difficulty in accessing key data on the specific releases and local dispersion. A strategy to use a combination of screening and detailed modelling has been developed as part of the second phase of this study.
7. Following the completion of the model evaluation undertaken in Phase 1 of this feasibility study, two options were identified for the strategic plan needed to predict the chemical density of Europe from emissions data. The options were: (1) a detailed modelling approach, and (2) a staged modelling approach, in which a screening model would be used to identify those emissions where further detailed modelling would be required. The staged modelling option is consistent with the tiered approach to modelling endorsed by the OECD for predicting the persistence and potential for long-range environmental transport of chemicals.
8. The study concluded that the second option (the staged approach) would offer the most cost-effective and efficient way forward. It makes use of the EUSES model for initial screening analysis of environmental concentrations resulting from EPER emissions. Comparison of the environmental concentrations predicted by the screening model with relevant environmental standards or other appropriate criteria would then be used to decide on the need for further assessment with more complex models requiring detailed spatially and temporally resolved input data.
9. The staged approach that underpins the strategy offers the advantages of cost effectiveness by only undertaking detailed modelling in cases where regional exceedances are predicted by the screening model and no alternative information sources are available.
10. The EU chemical risk assessment model EUSES was demonstrated to be suitable for undertaking the screening assessment as the first part of the staged modelling strategy by application to emissions of three contrasting chemicals listed in the EPER database. The chemicals were hexachlorobenzene, benzene and arsenic.

11. Scripts were written extract emission data from EPER and to run EUSES with each substance in turn and to generate map outputs of predicted local and regional environmental concentrations in air, surface water and (for arsenic) soil, allowing 'hot spots' to be identified.
12. The suitability of the EPER database as a source of data for concentration modelling has been assessed. The database allows information to be extracted readily to provide the input to chemical fate models by means of simple computer scripts. The database gives details of the geographical location of each source and so it is relatively straightforward to prepare maps of pollutant hot spots associated with EPER sources. The provision of the details of the geographical location of the site also greatly facilitates the extraction of site-specific environmental data for modelling from climate, land cover and river catchment databases.
13. To some extent, the EPER database duplicates the information already held in the EMEP large point source inventory. However, the EPER database provides information on emissions of a wider range of pollutants to both air and water; will be updated more frequently and includes a wider range of sources.
14. The EMEP large point source database provides information on the height of discharge above ground: this element is not available from the EPER database. It would be useful for the calculation of local and regional air concentrations, which are dependent on the height of emission.
15. We have considered whether the EPER data provides added value for both high and low resolution assessments. Our experience with hexachlorobenzene, benzene and arsenic modelling suggests that the EPER database does not contain sufficient information to allow a high-resolution detailed assessment to be carried out. For example, a detailed local assessment of air dispersion would require additional information about discharge stack heights and diameters, the temperature and velocity of discharge and local topographical details. In addition, detailed information on the composition of several chemicals that are reported as mixtures of related species is lacking. The format of the data is however suited to low resolution-screening assessments of large numbers of sources.
16. EPER may increase the usefulness of existing models on the (pan) European and regional level because it contains data for many more point sources than the existing data sources. Currently, it is often necessary to spatially disaggregate national or regional emission totals onto an emissions grid for modelling purposes. The EPER data will allow more precise allocation of emissions onto the model grid.
17. A simple addition to the EPER data return form is proposed that would allow information on local environmental concentrations to be submitted has been developed.
18. A draft work plan has been prepared to predict the chemical density of Europe from emissions of other substances listed in EPER. The first phase of this work, which would require two stages of EUSES screening modelling of selected substances, identification of appropriate assessment criteria and sensitivity and uncertainty analysis, is estimated to require about 80 mandays effort. The second phase would involve detailed spatially resolved modelling of substances found to exceed the relevant criteria in the first phase. Because of difficulties in gaining access to site-specific information needed to undertake accurate modelling of environmental concentrations, it is recommended that the assessment focus on modelling at the regional or greater geographical scale, rather than the local scale.
19. Overall, we believe that the staged proposed in this study will provide a feasible, cost-effective and efficient means of predicting the chemical density of Europe from industrial point-source emissions data. Further work would be required to predict chemical concentrations resulting from non-point sources, which in many cases are the dominant source of environmental releases, but where information on emission rates is currently much less available.

1 Introduction

The 2002 comprehensive assessment of the state of Europe's environment, presented to the ministerial environment conference in Kiev (May 2003) (1), drew attention in its chapter on chemicals to the lack of information on the distribution of chemicals in the environment. The report highlighted the uncoordinated nature of many monitoring programmes and the imbalance between the types of substances monitored. Monitoring programmes for chemicals in the environment have generally, for reasons of cost and technical complexity, been established with the aim of demonstrating compliance with international agreements, for example, those undertaken under the auspices of CLTAP (2) and OSPAR (3). However, there is currently little systematic monitoring data in the public domain for chemicals that have not so far become the subject of international control.

In the absence of measurements of chemical concentrations in environmental media, policy-makers and other interested parties make use of computer models that aim to calculate concentrations from data on the emissions of chemicals into the environment. The initial development of models to predict the environmental fate of chemicals may be traced back to the late 1970s, with the application of mass balance approaches and principles based on 'fugacity' advanced in pioneering research by Mackay, Thiobodeaux, Klöpffer and Frische, to mention but a few. The research area grew throughout the 1990s with numerous international conferences, workshops and seminars. The discovery of elevated concentrations of persistent organic pollutants (POPs) and mercury in remote Artic regions far from where these chemicals were released has further increased interest in models to predict regional and global movement of persistent and semi-volatile chemicals. The widespread application of chemical models has been made possible by the phenomenal rate of growth in computer performance over the past two decades, coupled with the improved accessibility of computers to non-specialist users, thanks to the fall in cost of computers and the availability of user-friendly software applications, such as Microsoft Excel® and other similar products. Continuing advances in computing power available to non-specialists, along with increasing concerns over possible harmful effects of traces of man-made chemicals in the environment and in human tissue, promise to ensure that environmental fate modelling continues to be a highly active area of research for years to come.

1.1 Purpose of the study

The purpose of this feasibility study is to develop a toolbox of available methodologies and a work plan for applying relevant models to substances reported under the European Pollution Emission Register (EPER) in order to predict the composition and distribution of these chemicals in the European environment — in effect, the 'chemical density' of Europe (4). The study aims to identify which of the available chemical models are sufficiently validated and accepted to be used in a policy context and which models are suitable for substances listed under EPER. The study will therefore focus specifically on models suitable for large industrial point source emissions, as opposed to diffuse sources, such as agricultural run-off, emissions from soils and releases from multiple small point sources, such as traffic and houses. The study also recognises that for some types of chemicals, notably the classical air pollutants of nitrogen oxides, sulphur dioxide, carbon monoxide and particulate matter (PM_{10} and smaller), and major water pollutants such as nitrogen, phosphorus and organic carbon, a number of models have already been established and are widely used in a policy context, such that

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(1) *Europe's environment: the third assessment.* European Environment Agency. Environmental assessment report No 10. Chapter 6: Chemicals.

(2) http://www.unece.org/env/lrtap/welcome.html.

(3) OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic. Meeting of the OSPAR Commission, Reykjavik: 28 June–1 July 2004. Agreement on Monitoring Strategies for OSPAR Chemicals for Priority Action. (Reference number: 2004-14). http://www.ospar.org/eng/html/welcome.html.

(4) The term 'chemical density' can have a variety of meanings, depending on the purpose for which the information is gathered. At its simplest level, we interpret the term to be equivalent to the concentration of a particular chemical species in the environmental media of interest. Alternative definitions may be needed for specific purposes but we have not attempted to identify them in this feasibility study.

further detailed evaluation is unnecessary. The study will instead place emphasis on models for manufactured chemicals and heavy metals.

1.2 EPER chemicals and modelling priorities

In July 2000, the European Commission adopted a decision on the implementation of a European pollutant emission register (EPER) (5) according to Article 15 of Council Directive 96/61/EC concerning integrated pollution prevention and control (IPPC) (6). The general purpose of the IPPC Directive is to reduce pollution by industry and to control emissions from larger facilities. EU Member States' governments are required to maintain inventories of emission data from specified industrial sources and to report emissions from individual facilities to the European Commission. The reported data are accessible in a public register (EPER), which provides information on releases of specified chemicals to air and water (both directly to receiving water bodies such as rivers, estuaries and coastal waters, and indirectly via a wastewater treatment plant) from major industrial activities. Member States submitted their first report in June 2003 relating to emissions in 2001. The next report will be delivered in June 2006 and will cover emissions in 2004.

There are some 50 chemicals currently listed in EPER. The number of facilities reporting releases of these chemicals to air and water (direct and via a wastewater treatment works) is shown in Table 1 and Table 2.

EPER can be considered as a first step towards the development of a fully integrated pollutant release and transfer register (PRTR) for Europe. A PRTR is a comprehensive version of a national emission inventory as referred to in the IPPC Directive. The parties to the Aarhus Convention (7) agreed in 1998 on the establishment of national PRTRs with *publicly accessible* emission data.

The European Community and its Member States (8) negotiated and finally signed the UN-ECE Protocol on PRTRs in May 2003. In order to ratify the protocol, the existing more limited EPER will be replaced by a comprehensive European PRTR. To simplify and streamline the reporting requirements, Council Directive 91/689/EEC on hazardous waste and Council Directive 96/61/EC concerning integrated pollution prevention and control have had to be amended and in addition a Council Decision on the conclusion of the UN-ECE protocol on PRTRs was also necessary to allow the Community to become a party to the protocol. Proposals (9) (10) to effect these measures have been adopted by the European Commission in October 2004.

As a result, the European PRTR (EPRTR) is expected to go on-line in 2009. It will then replace EPER, offering the following enhancements:

- Like EPER, it will provide information about emissions from specific industrial facilities and activities, and by country.
- While EPER reports on 50 substances emitted to air and water, the EPRTR will report on more than 90 substances released to air, water and land. The present register covers 56 industrial activities; the new one will cover 65. It will also have information on what the industrial installations do with their waste and wastewater.
- The reporting cycle will be annual instead of every three years.
- The EPRTR will include emissions from diffuse sources such as road traffic, aviation, shipping and agriculture as well as large industrial point sources currently listed in EPER.

Providing accessible information on chemical releases through PRTRs is an essential first step in allowing members of the public, policy-makers and other key groups with an indication of the types and

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(5) Commission Decision of 17 July 2000 on the implementation of a European pollutant emission register (EPER) according to Article 15 of Council Directive 96/61/EC concerning integrated pollution prevention and control (IPPC) (notified under document number C(2000) 2004). http://europa.eu.int/servlet/portail/RenderServlet?search=DocNumber&lg=en&nb_docs=25&domain=Legislation&coll=&in_force=NO&an_doc=2000&nu_doc=479&type_doc=Decision.

(6) http://europa.eu.int/comm/environment/ippc/index.htm.

(7) UNECE Aarhus Convention on access to information, public participation in decision-making and access to justice in environmental matters. http://www.unece.org/env/pp/.

(8) With the exception of Slovakia and Malta.

(9) Proposal for a regulation of the European Parliament and of the Council concerning the establishment of a European pollutant release and transfer register and amending Council Directives 91/689/EEC and 96/61/EC Brussels, 7.10.2004, COM(2004)634 final 2004/0231 (COD).

(10) Proposal for a Council Decision on the conclusion, on behalf of the European Community, of the UN-ECE Protocol on pollutant release and transfer registers. Brussels, 6.10.2004, COM(2004)635 final, 2004/0232 (CNS).

Table 1 Number of facilities reporting releases to air in EPER in 2001

Chemical release	Number of reported releases
Ammonia, NH_3	3 025
Nitrogen oxides, NO_X	2 086
Carbon dioxide, CO_2	1 507
Methane, CH_4	1 265
Sulphur oxides (SO_X)	1 257
Non methane volatile organic compounds (NMVOC)	773
PM10 (Particulate matter less than 10 μm)	531
Nickel and its compounds	475
Carbon monoxide, CO	471
Chlorine and inorganic compounds (as HCl)	431
Dinitrogenoxide (N_2O)	405
Mercury and its compounds	346
Zinc and its compounds	345
Lead and its compounds	280
Cadmium and its compounds	259
Fluorine and inorganic compounds (as hydrogen fluoride)	238
Arsenic and its compounds	227
Benzene	211
Chromium and its compounds	209
Copper and its compounds	177
Dichloromethane (DCM)	144
Trichloroethylene (TRI)	105
Hydrofluorocarbons (HFCs)	94
Polycyclic Aromatic Hydrocarbons (PAH)	88
Dioxins and furans (PCDDs and PCDFs)	86
Dichloroethane-1,2 (DCE)	41
Tetrachloromethane (TCM)	35
Hydrogen cyanide (HCN)	35
Tetrachloroethylene (PER)	34
Perfluorocarbons (PFCs)	29
Sulphur hexafluoride (SF6)	23
Tetrachloromethane (TCM)	19
Trichlorobenzenes (TCBs)	2
Pentachlorophenol (PCP)	1
Trichloroethane-1,1,1 (TCE)	1
Total	**15 255**

quantities of chemicals to which they are exposed via the environment. However, it is the degree of exposure to a harmful substance that determines the level of risk posed — not just the quantity released because chemicals vary greatly in their toxicity, persistence and environmental behaviour. The role of environmental modelling of chemicals is to predict the concentrations in environmental media over space and time that result from a given release or collection of releases. This information may be considered to represent the 'chemical density' of a region. By taking account of the distribution and behaviour of sensitive receptors (such as humans, other species, sensitive ecosystems, etc.) the level of exposure may then be calculated. Comparison of the exposure level with safe levels for particular impacts (such as specific health end points, harm to sensitive species, etc.) provides the basis of

Table 2 Number of facilities reporting releases to water in EPER in 2001

Chemical release	Number of reported releases*	
	Direct	Indirect
Total organic carbon (TOC)	613	803
Zinc and its compounds	527	188
Nickel and its compounds	465	269
Copper and its compounds	343	120
Nitrogen, total	297	153
Lead and its compounds	288	101
Phosphorus, total	270	304
Chromium and its compounds	231	130
Arsenic and its compounds	229	69
Phenols	200	147
Chlorides	186	40
Cadmium and its compounds	172	41
Fluorides	172	32
Mercury and its compounds	160	41
Halogenated organic compounds (AOX)	132	33
Cyanides, total CN	72	30
Benzene, toluene, ethylbenzene, xylenes (as BTEX)	50	54
Polycyclic aromatic hydrocarbons (PAH)	46	19
Dichloroethane-1,2 (DCE)	37	14
Dichloromethane (DCM)	33	28
Organotin compounds	7	2
Hexachlorobutadiene (HCBD)	5	1
Hexachlorobenzene (HCB)	4	
Hexachlorocyclohexane (HCH)	3	
Chloro-alkanes (C10–13)	1	3
Brominated diphenylethers		1
Total	**4 543**	**2 622**

Note: * Sorted according to descending order of direct releases. Indirect releases are where the release takes place to a wastewater treatment plant.

risk assessment methodology that underpins policymaking in this field. Where it is possible to estimate a monetary cost of an impact (such as the cost of increased morbidity or mortality, damage to agricultural crops, etc.) and there is an established exposure — impact relationship, then economic costs of policy options that reduce exposure may be compared with the benefits due to reduced impacts on an objective economic basis. This is the principle underpinning models such as RAINS (11) that are playing an increasing role in quantifying the economic costs and benefits of air pollution policy. Both risk evaluation and economic assessment depend on knowledge of chemical concentrations in the environment. The focus on this study is on how best to provide the link between emissions and environmental concentrations.

The basic aim of modelling is to predict the environmental concentrations of a substance following its release. The type of model that may be required for this purpose depends strongly on the properties of the chemical concentrated and the medium (air, water, soil, etc.) into which it is released. Furthermore, the choice of model also reflects the purpose for which the information is being gathered. For example, 'screening' type models can be used to predict environmental

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(11) http://www.iiasa.ac.at/rains/Rains-online.html?sb=8.

concentrations in environmental media averaged over local, regional or continental scales, but taking no account of variations within particular areas due to geographical, meteorological or hydrological factors that determine the dispersion of the chemical. Such screening models, when based on realistic worst-case assumptions about the environmental persistence and dispersion of a chemical following release may be used to give assurance that relevant environmental quality standards are being achieved and that the risk of adverse effects are acceptably low. Models of this type are used for chemical risk assessment for new and existing chemicals, by regulatory authorities to establish emission discharge consent levels, and by industry to give assurance of compliance with environmental standards. The outcome of such modelling can also be used to indicate when further, more detailed, modelling is needed and where modelling results may need to be backed up with specific measurements.

Models may also be used to compare the contribution of a particular emission source on the overall environmental concentration of the chemical in various media from all other sources, bearing in mind that for some chemicals, natural sources may also be important, along with other man-made sources such as traffic, domestic emissions and releases from facilities not regulated under IPPC. The calculation of the 'process contribution' is of interest as it helps to indicate the headroom that is available between a relevant environmental quality standard and actual concentrations, which will need to be taken into account in setting permit conditions for further facilities.

The properties and release route of a chemical play a major role in determining its environmental distribution and hence the types of models that need to be brought into play. Chemicals released into the air and which are removed fairly rapidly (by decomposition or deposition processes) do not generally require the use of large-scale multimedia models to predict their distribution. This can be done using one of a number of well-established local air dispersion models. These will, when provided with information on the release conditions (such as stack height, exit temperature of the gas etc.), topographical features (such as slope, surface roughness, hills and other obstacles etc.) and prevailing meteorological conditions (wind velocity fields, precipitation, etc.) allow the detailed spatial distribution of concentrations to be calculated, along with relevant statistics such as mean and confidence intervals of the calculation. The output from such models is usually available in graphical form, such as contour maps of concentration, when the model is coupled with a GIS database.

A similar approach may be taken with chemicals released to water. Models of surface water releases take account of dilution and dispersion of the chemical in the receiving water, its decomposition by chemical and biological processes, sorption and transport in sediments and predict the resulting concentration in the water column, sediment and biota. For volatile chemicals, the models also need to take account of transfers from water to air by evaporation. Detailed graphical output of predicted concentrations downstream of a release is possible where GIS data are available for particular watershed systems.

Many industrial releases of chemicals to water are not made directly to the receiving water itself, but instead go via a wastewater treatment plant. These come in a variety of designs, from simple precipitation plant to multi-stage anaerobic/aerobic processing. Models are needed that determine how the inflowing chemical will be partitioned between the various off-streams from the plant: namely in releases to the air, in the treated effluent and in sewage sludge and the amount removed through decomposition. The use of sludge as a soil conditioner transfers persistent pollutants from the wastewater plant to land, and hence to crops and food animals.

Models of greater complexity are required for semi-volatile chemicals that can move between the atmosphere and surfaces and whose resistance to decomposition allows them to travel for great distances. The classic examples of such chemicals are certain POPs and mercury. When released into the atmosphere, these chemicals undergo a cycle of repeated deposition and resuspension, a sort of global distillation that transfers them from mid latitudes towards the colder regions, such as the Arctic. As these substances are highly lipophilic, they accumulate in biota, particularly in fat, to the extent that they may pose a significant health threat to indigenous people who rely on oily fish and marine mammals for the major part of their diet. Models used for predicting concentrations of these types of chemicals generally include a detailed treatment of processes governing long-range transport through the atmosphere, including deposition and resuspension processes, but they also need to take account of transfers between all relevant environmental compartments, including land, sea and (in some cases) ice fields. These multimedia models are used to predict regional or continental patterns of concentration in various environmental media and biota and deposition rates. Multimedia models may also be large scale in the temporal domain: the persistence of chemicals of this type means that significant levels remain for decades after primary emissions have been eliminated and that levels in soils may serve to top-up atmospheric concentrations for many years.

1.3 Structure of this report

Section 2 describes the methodology, focussing on the approach adopted for model evaluation in Phase 1.

Section 3 reports the outcome of the Phase 1 model evaluation. It reviews a selection of models developed for local air quality assessment, acidification and eutrophication (caused by emissions of sulphur dioxide, nitrogen oxides and ammonia), photochemical oxidant formation, and surface water and sewage treatment plant models. It includes an assessment of range of models of varying complexity, from simple screening type models with minimal input data requirements and highly detailed models producing output with a high degree of spatial and temporal resolution. The final part of Section 3 outlines a series of conclusions based on the model evaluation.

Section 4 reports the work undertaken under Phase 2 of the feasibility study. It first describes the strategic plan to be followed (Task 8) for predicting the chemical density of Europe from emissions data. It then reports the results of model runs designed to test the strategy (Task 6) and, from the information so obtained, presents a draft work plan for the application of the strategic approach to EPER release data. The conclusions from Phase 2 of the study are then presented.

Appendix 1 contains the technical specification of the project drawn. Appendix 2 lists the delegates at the brainstorming meeting held in March 2005. Appendix 3 lists comments on the draft final report from experts at an international summer school on chemical modelling, and finally Appendix 4 presents the proceedings of an expert workshop reviewing the project that was held in Copenhagen on 16 August 2005.

2 Methodology

In summary, the work consists of the following tasks, broken down into two phases:

Phase 1

1. Identify available models.
2. Verify their status of validation and general acceptance.
3. Evaluate selected models for their ability to provide information on the spatial distribution of chemicals in the different environmental media in the geographical area of the EEA member and participating states.
4. Scan models and provide information on the time and spatial scale they cover, provide expert judgement on the resolution needed for assessment of (pan) European, national, regional or local pollution and describe model characteristics for each level.
5. Identify which models are applicable to EPER substances.

Phase 2

6. Run one or more models for a test substance using EPER database releases to map chemical concentrations, identify 'hot spots' assess usefulness of EPER data for this purpose, and compare predicted concentrations with measured values, if available.
7. Draft a work plan to extend Task 6 to all relevant models identified in Task 5.
8. Develop a strategic proposal on how these models and derived data can be used to estimate the chemical density in the European environment based on emission data.
9. Summarise the findings in the final report.

In Phase 1, Tasks 1 and 2, which deal with the identification of available models and verification of their status and general acceptance, were undertaken in parallel. Similarly, Tasks 4 and 5 were undertaken as part of the model evaluation performed in Task 3. Models were identified from the consultant's knowledge and experience in this field, supplemented by Internet and literature searches and contacts with researchers. An important element of this stage of the work was a brainstorming meeting, held at the consultant's premises on 2 March 2005. The purpose of the meeting was to assist in identifying models suitable for predicting environmental concentrations of chemicals from emissions data held in EPER, verifying their status, identifying the principal purposes of the model toolbox and the criteria proposed by the consultants for model evaluation. Some twenty experts from industry, regulators, policy-makers and the research communities attended the one-day meeting, which was organised in a workshop style. Delegates are listed in Appendix 2.

The detailed findings from the brainstorming meeting were reported in the meeting minutes. The main conclusions are summarised in Box 1. In line with these conclusions, in particular numbers 3 and 11, the study has placed greatest emphasis on the evaluation of multimedia models developed for predicting chemical distribution in the environment, particularly of persistent chemicals with the potential for long-range transport.

2.1 Model evaluation criteria

The models were evaluated according to a framework presented and endorsed at the brainstorming meeting. The criteria are shown in Box 2. Please note that in general, the price of commercially available software (part of evaluation criterion 1) may vary with supplier, model release, market conditions and the status of the purchasing body (e.g. commercial consultants, academia or other not-for-profit organisations). We have therefore not provided price information as part of the assessment. However, from our investigations we conclude that single user licences for most commercially available software may typically be purchased for around EUR 1k. Regarding criterion number 3, few if any models evaluated make explicit reference to having been produced to a recognised software quality standard, such as ISO 9001 TickIT, so in most cases it has not been possible to determine this aspect of quality.

Box 1 Conclusions from the brainstorming meeting on 2 March 2005

1. The main users of models for use with emission inventories were identified as regulators, industry, policy-makers and researchers. They use models for a range of purposes, including setting release limits and permit conditions, predicting the effects of releases (permitted and non-permitted) on environmental concentrations of chemicals, demonstrating regulatory compliance, showing compliance with international obligations and undertaking policy and regulatory evaluation, amongst other things.
2. The delegates did not explicitly consider uses by citizens groups and NGOs. However, the larger NGOs, at least, would be expected to have access to environmental models with which to undertake their own evaluations of releases and regulatory and policy assessment. The review of the US EPA study on uses of toxic release inventories provided in the delegates briefing pack, it appeared that there were few instances where models had been used by citizens groups to derive information on environmental concentrations of chemicals from the basic release data given in the inventories. The availability of free access models downloadable from the Internet may change this position. However, regulators and industry are understandably wary of new and unproven models, or indeed established models being misused, that could undermine the permitting process and compliance demonstration.
3. Overall, delegates did not identify major gaps in the availability of environmental models for established purposes relating to types of chemical that are already controlled through existing legislation and international agreements. The main types of substances in this category includes substances that are not deliberately manufactured, such as some POPs (the focus of development of large-scale multimedia models), acid gases, heavy metals, fine particulate matter; and VOCs, for which both regional and local scale air pollution models are available. There are several very well established local air quality models that are widely used. It takes 10–15 years for models to attain this level of acceptance. Delegates also identified several studies where alternative models have been compared.
4. There appeared to be fewer models dealing with degradable manufactured chemicals that do not fit into the above categories. Some air pollution and multi-media models do not allow for decomposition processes. This can be acceptable in screening models, particularly at local scales, where it will usually result in over-estimation of environmental concentrations, but is more problematical with large-scale multimedia models. Two further difficulties with these types of model were also identified. Firstly, the treatment of sea water as a single box makes it verification of the model through monitoring very difficult. Secondly, models tend not to take account of ionisation state, which will of course control key drivers such as vapour pressure and partition coefficient for polar molecules.
5. Aquatic and soil models tend to be very much more dependent of site-specific input data, through their very nature, than air models. Apparently different models may use the same modelling approach or algorithms. This needs to be taken into account in the evaluation process.
6. Overall, delegates support the approach to model assessment provided in the briefing pack, but emphasising the need for transparency and objectivity in the process. Emphasis was also given to the need to record the underlying principles of operation of models, to include evidence of numerical testing and to also categorise models for scanning and more detailed analysis purposes.
7. Delegates considered that as part of the model evaluation process, it would be useful to benchmark models producing detailed spatially disaggregated concentration data at various scales (e.g. ADMS, EMEP) against EUSES, the established screening model, for specific examples of chemicals.
8. Some delegates considered that there is a need to improve the connectivity between models operating at the regional and local scales. In addition, some delegates noted that although detailed hemispheric models are available, there is a lack of models at this scale that could be used for scoping studies.
9. Models should also produce an indication of the uncertainty of their outputs — this could be done through scenario analysis or Monte-Carlo approach.
10. A major source of uncertainty in modelling environmental concentrations of chemicals lies in both detailed information on the release and in the metadata (geographical, meteorological, hydrological factors, etc.) that determine dispersion and distribution following release. Emissions inventories such as EPER provide data on releases in unit mass per year — details of the timing of release (day, night, batch, continuous etc.), stack discharge heights, etc., are lacking. Similarly, finer detail is required on other metadata (from meteorological, hydrological, geographical and soils databases) if the potential for finer-scale spatial and temporal prediction of detailed models is not to be lost through uncertainly in input data.
11. It is important in the present study to define and then concentrate on a small number of specific uses for chemical models and to avoid taking too broad an approach that may hinder the efficient use of resources.

2.2 Contents of a model toolbox

Given that the stated purpose of the feasibility study is to 'develop a toolbox of available methodologies' that could be used to predict the chemical density in Europe from EPER substances, it is helpful to consider what types of methodologies and models should be available in such a toolbox.

From considerations of the specific purpose of this study and the overall objectives of the EEA in making environmental information widely available and in promoting improved environmental performance, we have considered a number of attributes that such toolbox should have. In addition to the obvious needs for scientific validity there are also a number of administrative and policy related issues that must also be considered, as indicated below: the properties of a useful toolbox of models are shown in Box 3. These provide a useful point of reference for the strategy and work plan for the future development of this work, described in Phase 2 of this study (in Section 4).

Box 2 Model evaluation criteria

1. **Availability** of the model — is it a commercial product? If so, what is its licence cost? Is it available as a web down-load? Is it available free of charge? What use restrictions (if any) are applied by the owners of the intellectual property rights?
2. **Peer review status** — what evidence is there that the model has been subject to independent peer review for its intended purpose? Is the model based on accepted scientific methodologies? — if not, has any novel approach been peer-reviewed? Is there any formal or informal endorsement from authoritative bodies which have used the model?
3. **Quality issues** — what evidence is there for calibration and validation of the model's output in its intended application? How well does the model predict measured concentrations (if available)? Has the model been developed using a recognised quality assurance standard for software (egg ISO 9001 TickIT)?
4. **Adequacy of information** — is there a full description available stating the input parameter and variables required, the mode of operation of the model, access to the code and algorithms used, the nature of output data, is it available as graphical (map or chart) outputs, data files etc.?
5. **History of usage and development** — is there evidence that the model is currently in use for its intended purpose? Has it been superseded by later versions or types? Is it currently being maintained, developed and supported?
6. **Resource requirements** — what computational and human resources are required to operate the model? Can it be run on a 'typical' PC or are special resources required? How long does a model run typically take on an appropriate type of computer? What level of training and specialist knowledge is required for users? Is the model 'user-friendly'?
7. **Availability of input data** — does the model accept annual emission data per facility as recorded in EPER or other release inventories? If not, what level and nature of pre-processing is required to provide the input data in the required form? What other inputs may be required that are not presently in release inventories but which could be considered in the future (egg stack height data, information on temporal patterns of release, plume rise parameters, local topology and meteorology, etc.)?
8. **What modelling approach is used** — egg Gaussian plume, Lagrangian, Eulerian, fugacity distribution modelling, empirical or semi-empirical approaches?
9. **For which groups of substances is the model intended** — egg persistent organic chemicals (e.g. POPs and POP-like substances), heavy metals, acid gases, VOCs and other types of substance? Which new substances likely to be reported in EPER in 2009 will the model address?
10. **Nature of model outputs** — e.g. does the model produce map outputs, other graphical outputs, type of output file (e.g. CSV, XML, spreadsheets etc.). How suitable is the output for use in fate modelling for risk assessment, in compliance with the technical guidance documents?

Box 3 Properties of a model toolbox

Applications

- Tools are required that will allow EPER emissions to be used, with appropriate supporting data, to predicted environmental concentrations of chemicals.
- The principle environmental media of interest are air, surface water, sediment, soil and vegetation.
- The spatial and temporal scales on which the information is provided must be appropriate to the environmental properties of the chemicals in question.
- The models will allow concentrations from EPER emissions to be compared on an installation-by-installation basis, groups of installations and with background concentrations where data are available.
- The information should be presented in appropriate graphical/map format to allow these comparisons to be made.
- The analysis must cover the entire area of EEA countries.

Scientific validity

- The approach adopted must be based on sound science, using models that have been subject to rigorous peer review and with a track record of application in the relevant field.
- Where uncertainties exist, these must be unambiguously stated.
- Well-proven models with an established record of use will be preferred over novel but perhaps less proven approaches.

Transparency

- The following information must be accessible to users of the model outputs:
  - input data;
  - underlying assumptions;
  - calculation protocols.

Administrative and policy considerations

- The toolbox must not require changes in legislation or policy for it to be successfully implemented.
- The methodologies must not place a disproportionate administrative or cost burden on the user such as EEA or other public or private bodies for developing, maintaining and providing input information.
- The output from the toolbox — in terms of predicted environmental concentration — must be presented in such a way as to minimise the possibility of spurious challenges to industrial site 'permit to release' conditions.
- Model outputs must be amenable to revision as more accurate information is made available.

As a driver for environmental improvement

- Public access to environmental concentration data will allow comparison between facilities and should increase pressure for environmental improvements and /or submission of more accurate concentration data by industry. This pressure will be greatest those for facilities causing the highest environmental concentrations.

3 Phase 1 — Model evaluation

3.1 General aspects

This section describes the outcome of the model evaluation undertaken in Phase 1. It first outlines some general considerations on spatial and temporal scales required for certain types of chemical. It then deals with local scale air pollution models, multimedia models for both screening purposes and for producing spatially resolved concentration maps and lastly models for surface water and sewage treatment works. It considers the suitability of models for use with particular EPER substances, the adequacy of the data in EPER for modelling purposes, and the required additional input data.

3.1.1 Spatial and temporal aspects of chemical modelling

The temporal and spatial scales appropriate to modelling the concentration of a particular chemical following its release depends to a large extent on persistence of the chemical (i.e. resistance to decomposition) and mobility. As the atmosphere is the environmental medium in which mass flows occur most rapidly on a global scale, mobility is generally reflected by volatility. It therefore follows that volatile chemicals have the greatest potential to be transported over large distances, provided they are sufficiently persistent to avoid decomposition. The spatial scale of models appropriate to different types of chemicals may therefore be envisaged as being mapped onto a simple persistence-mobility matrix, as shown in Figure 1.

Low persistence chemicals generally require modelling on a local scale, close to the site of release, because the substances will have mostly degraded before they can travel further. Similarly, low mobility chemicals will also require local modelling. Chemicals of intermediate mobility (such as semi-volatile POPs, mercury), which are also persistent, will require models operating at a regional to global scale to capture concerns over their distribution. Highly mobile and persistent chemicals require global scale modelling. Examples of these chemicals include greenhouse gases and chemicals that destroy stratospheric ozone. Models for these types of impact are outside the scope of the present study because there is generally no need to localise these impacts to any particular emission source.

Chemical decomposition processes are usually modelled by first order or pseudo-first order kinetics and are based on the assumption that the products of decomposition are themselves of no concern, compared with the substance initially released. Generally this assumption holds true, although in some cases, for example, certain pesticides where the decomposition products are also harmful, special considerations may be built into the models on a case-by-case basis. In other instances, for example, with heavy metals, decomposition processes play no part, although there may be other processes that need to be taken into consideration that affect the mobility and bioavailability of the substance in question.

3.2 Air quality models

Various types of model have been developed for predicting the concentrations of chemicals emitted into the atmosphere in the locality of emission sources. A selection of well-established local air pollution models is reviewed in the following section. Other types of model have been developed to take account of the impact of the emitted chemical in terms of secondary pollutants and their impacts that are formed from the chemical initially released. The prime examples of these secondary pollutants are ozone and other harmful oxidants formed in polluted air by chemical and photochemical reactions between oxides of nitrogen and volatile organic compounds, and the deposition of acids and nutrients formed from emissions of sulphur oxides, oxides of nitrogen and ammonia. Models dealing with photochemistry and acid deposition are also considered in Sections 3.2.2 and 3.2.3. In addition, a number of large-scale (regional, continental and hemispheric) atmospheric models have been applied used alongside multimedia models (12) for assessing the long-range transport of some persistent air pollutants. It makes sense therefore to discuss these models in the context of multimedia models, in Section 3.3.4.

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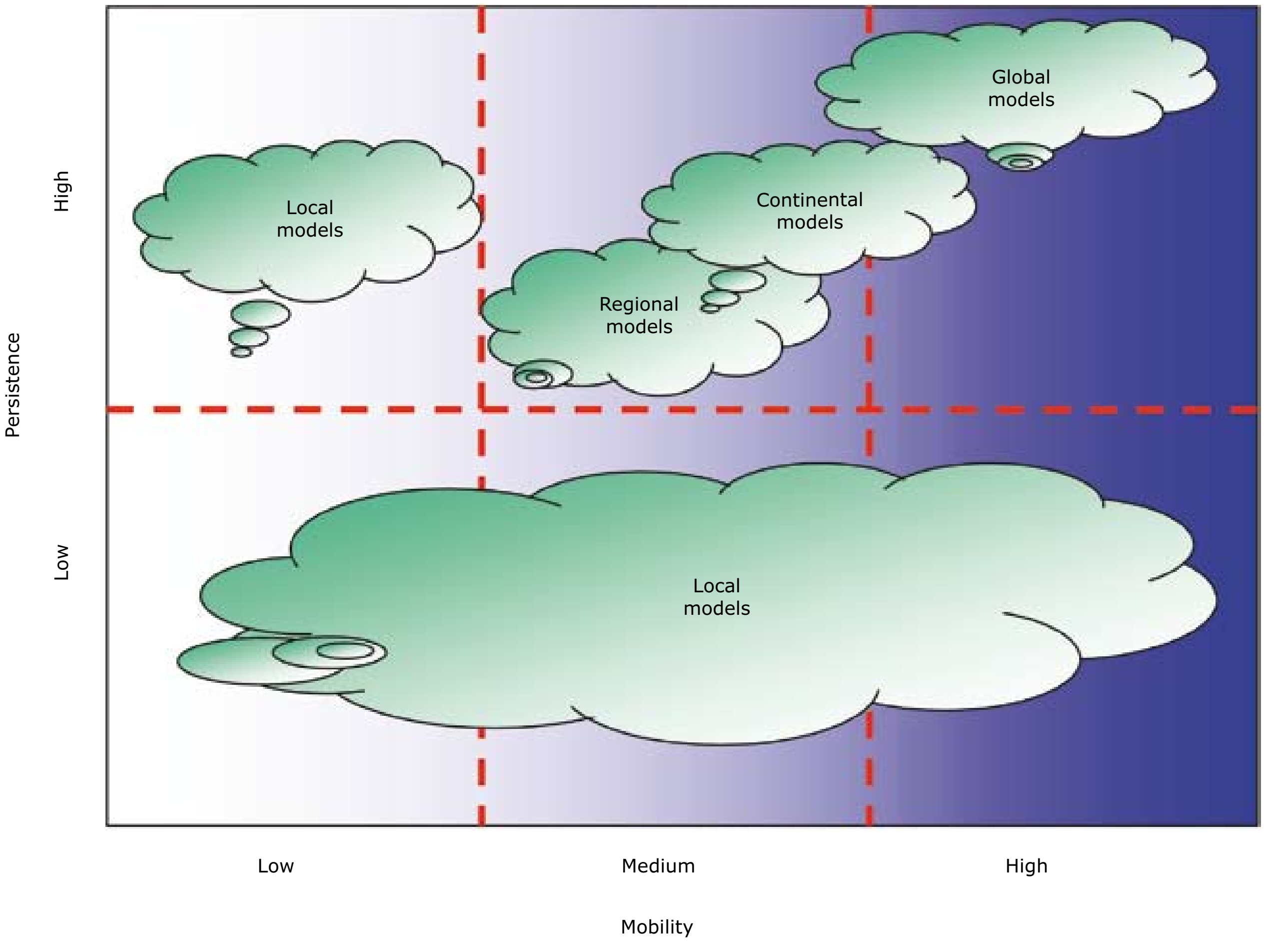
(12) Such as DEHM, ADOM, Hysplit-4 and CMAQ-Models 3.

Figure 1 Spatial scales for chemical modelling



3.2.1 *Local air pollution models*

Local scale air pollution models are used to assess the impact of emissions of pollutants to the atmosphere on ground-level concentrations in the vicinity of the emission source. Various types of emission source are modelled including industrial stack discharges, fugitive emissions from factories, diffuse emissions from areas such as landfill sites, and traffic emissions from roads.

Most of the substances in the EPER database have a detrimental effect on local air quality, human health and vegetation. Adverse effects on human health may arise from chronic exposure over the long term or from acute exposure over the short term. European Council Directives have established air quality standards and objectives for various pollutants within the EPER database. Environmental assessment levels for many other pollutants are also widely applied. Local scale air pollution models are widely used to assess potential exceedence of these benchmarks.

There are a large number of established models used for local air quality assessment available. Their state of development and an overview of their application are reviewed in an EEA technical report (EEA, 1996) ([13]), to which the reader is referred for further detailed information. The models listed in Table 3 are applicable to point source emissions listed in the EPER database. Various other models are also used to assess the impacts from traffic emissions from roads: these models have not been considered here, but are included in the database.

Modelling approaches
Local-scale air pollution models may be placed in two broad categories:

- Eulerian (plume and puff) models;
- Lagrangian particle dispersion models.

([13]) *Ambient air quality, pollutant dispersion and transport models.* Topic report No 19/1996, European Environment Agency. http://reports.eea.eu.int/92-9167-028-6/en/tab_abstract_RLR.

Table 3 List of typical local air pollution models

Model	Information sources/URL
ADMS	http://www.cerc.co.uk/
AERMOD	http://www.epa.gov/scram001
AEROPOL	http://pandora.meng.auth.gr/mds/showlong.php?id=100
AirQUIS-EPISODE	http://www.nilu.no/airquis/models_dispersion.htm
AUSTAL2000	http://www.austal2000.de
DIPCOT	http://milos.ipta.demokritos.gr/DIPCOT.htm
DISPERSION21	http://www.smhi.se/foretag/m/dispersion_eng.htm
EK100W	http://pandora.meng.auth.gr/mds/showlong.php?id=37#d_1
GRAL	http://pandora.meng.auth.gr/mds/showlong.php?id=133#d_14
HNS-TRANSMISSION	http://www.levegokornyezet.hu/04.htm http://pandora.meng.auth.gr/mds/showlong.php?id=48#d_1
IFDM	http://pandora.meng.auth.gr/mds/showlong.php?id=50#d_1
INPUFF	http://pandora.meng.auth.gr/mds/showlong.php?id=51
ISCST	http://www.epa.gov/scram001
LASAT	http://www.janicke.de/lasat/e_lasat.htm
MODIM	http://pandora.meng.auth.gr/mds/showlong.php?id=110#d_14
NORMAL	http://pandora.meng.auth.gr/mds/showlong.php?id=67#d_1
OML	http://www2.dmu.dk/1_viden/2_Miljoe-tilstand/3_luft/4_spredningsmodeller/5_OML/OML-multi_broch_en.pdf http://pandora.meng.auth.gr/mds/showlong.php?id=112#d_1
OND-86	http://pandora.meng.auth.gr/mds/showlong.php?id=71
ONM9440	http://pandora.meng.auth.gr/mds/showlong.php?id=72
PLUME/PLUME Plus	http://pandora.meng.auth.gr/mds/showlong.php?id=77#d_1
POLGRAPH	http://pandora.meng.auth.gr/mds/showlong.php?id=78#d_1
PPM	http://pandora.meng.auth.gr/mds/showlong.php?id=114#d_1
SPRAY	http://www.aria-net.it/PDF/e_spray3.pdf http://pandora.meng.auth.gr/mds/showlong.php?id=87
STACKS	http://www.kema.com/consulting_services/power_generation/environment/environmental_services/http://pandora.meng.auth.gr/mds/showlong.php?id=88#d_1
SYMOS-97	http://pandora.meng.auth.gr/mds/showlong.php?id=119#d_1
ScalExNeuro	http://pandora.meng.auth.gr/mds/showlong.php?id=92#d_1
UDM-FMI	http://pandora.meng.auth.gr/mds/showlong.php?id=121#d_1
VADIS	http://pandora.meng.auth.gr/mds/showlong.php?id=122#d_1

These modelling approaches are described in further detail in Box 4 and Box 5.

Model features

Point source emissions from industrial stacks usually have significant upward momentum and buoyancy, so that the effective height of emission may be considerably greater than the physical stack height. Most models take account of this plume rise using various empirical formulae (e.g. ISCST, OML): other models (e.g. ADMS) calculate plume rise by numerical solution of the integral conservation equations for the fluxes of mass, momentum and heat in the rising plume.

Plume models generally assume flat terrain throughout the model domain. In practice this assumption is reasonable provided that terrain slopes are generally less than one in ten. Under these conditions the wind streamlines effectively follow the terrain. For more complex terrain, it is necessary to calculate the wind field separately prior to the dispersion calculation: some models provide an integrated package to calculate both the wind field and the pollutant dispersion. For example, ADMS and VADIS include separate modules to calculate the airflow pattern over hills and the pollutant dispersion.

Box 4 Eulerian modelling approach

The majority of local scale air pollution models treat the atmosphere as a continuum, with wind speed and pollutant concentrations varying smoothly throughout the model domain. Plume and puff models are based on the principle of mass conservation of pollutants. Consider a volume element in the atmosphere, where gases containing a pollutant *A* are flowing into the element. An instantaneous mass balance on the component *A* leads to the following differential equation:

$$u_x \frac{\partial c_A}{\partial x} + u_y \frac{\partial c_A}{\partial y} + u_z \frac{\partial c_A}{\partial z} + \frac{\partial c_A}{\partial \theta} + c_A \left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) - D_{AB} \left(\frac{\partial^2 c_A}{\partial x^2} + \frac{\partial^2 c_A}{\partial y^2} + \frac{\partial^2 c_A}{\partial z^2} \right) + \Lambda_A c_A - R_A = 0$$

where

U_X, U_Y, and U_Z are in the wind speeds in the x and y horizontal dimension and z vertical dimension;
C_A is the concentration of A;
D_{AB} is the molecular diffusivity of A through medium B;
Λ_A is the wet scavenging coefficient;
R_A is the rate of production of A by chemical reaction;
θ is time.

This differential equation is simplified in various ways in most models used for assessing local scale air pollution. All the models considered assume that the turbulent motion in the atmosphere can be resolved into a fluctuating component superimposed on the general mean flow. Thus the instantaneous components of the wind velocity along the x-axis may be defined as:

$u = \bar{u} + u'$

where the over bar refers to the mean velocity and the prime refers to the instantaneous fluctuation from the mean. It is also generally assumed that the rates of molecular diffusion are small compared with the rate of pollutant dispersion by turbulence.

These assumptions lead to the following simplification of the mass conservation equation:

$$\bar{u}_x \frac{\partial \bar{c}_A}{\partial x} + \bar{u}_y \frac{\partial \bar{c}_A}{\partial y} + \bar{u}_z \frac{\partial \bar{c}_A}{\partial z} + \frac{\partial \bar{c}_A}{\partial \theta} + \left(\frac{\partial \langle u'_x c'_A \rangle}{\partial x} + \frac{\partial \langle u'_y c'_A \rangle}{\partial y} + \frac{\partial \langle u'_z c'_A \rangle}{\partial z} \right) + \Lambda_A \bar{c}_A - R_A = 0$$

where the angled brackets denote time-averaged values.

The eddy flux terms (in brackets) may be replaced by various empirical functions, the simplest of which is the gradient transfer form:

$$K_y \frac{\partial c_A}{\partial y} = -\langle u'_y c'_A \rangle \text{ etc.}$$

Substituting the gradient transfer equation into the mass conservation equation gives:

$$\bar{u}_x \frac{\partial \bar{c}_A}{\partial x} + \bar{u}_y \frac{\partial \bar{c}_A}{\partial y} + \bar{u}_z \frac{\partial \bar{c}_A}{\partial z} + \frac{\partial \bar{c}_A}{\partial \theta} - \left(\frac{\partial}{\partial x}\left(K_x \frac{\partial c_A}{\partial x} \right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_A}{\partial y} \right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_A}{\partial z} \right) \right) + \Lambda_A \bar{c}_A - R_A = 0$$

Over time periods of approximately one hour or less it is possible to assume that the wind field is effectively constant. Plume models assume that the concentration approaches steady state for a continuously emitting source. Puff models; on the other hand assume that the duration of the emission is short so that the pollutant is advected with the mean wind.

The plume and puff models assessed assume that the mean vertical and crosswind wind speeds, *uz* and *uy* are effectively zero. Plume models also assume that the dispersion along the x-axis, in the direction of the wind is also zero. If it is then assumed the dispersion coefficients, K_y and K_z are constant and uniform, then it is possible to derive an analytical solution for plume models, taking account of upper and lower boundaries representing the ground and the top of the atmospheric boundary layer or inversion layer:

$$c_A = \frac{Q}{2\pi \sigma_y \sigma_z u} \exp\left[-\frac{y^2}{2\sigma_y^2} \right] \sum_{N=-\infty}^{+\infty} \left[\exp\left(-\frac{(h_s - z + 2NH)^2}{2\sigma_z^2} \right) + \exp\left(-\frac{(h_s + z + 2NH)^2}{2\sigma_z^2} \right) \right]$$

$$\sigma_y^2 = \frac{2K_y x}{u}$$

$$\sigma_z^2 = \frac{2K_z x}{u}$$

Box 4 Eulerian modelling approach — contd

where Q is the rate of emission from a point source, hs is the height of the emission source above ground, H is the height of the inversion layer above ground. Similar analytical solutions have also been developed for puff models. This equation forms the basis for Gaussian plume models. Older models of this type (e.g. R91, ISCST) use empirical formulae based on the analysis of field data to estimate the dispersion coefficients σ_y and σ_z as a function of distance from the source and of the atmospheric conditions. More recently, 'new generation' plume models (e.g. ADMS, AERMOD, OML) have estimated the dispersion coefficients from the meteorological conditions on the basis of Monin-Obukhov similarity theory. Alternative analytical solutions, for example those assuming that K*z* may be represented by a power law function of height above ground are also possible (e.g. OMD-86).

Box 5 Lagrangian modelling approach

Lagrangian particle dispersion models represent the pollutant emission as a stream of discrete particles. The motion of each particle affected by the mean wind field and the turbulent fluctuations in wind velocity is followed throughout the model domain. By following large numbers of particles it is then possible to estimate pollutant concentrations from the density of particles at each location. The turbulent motion of each particle is assumed to follow Langevins equation. In finite difference form, Langevin's equation in the x-dimension may be written as:

$$u'(t) = \left(1 - \frac{\Delta t}{T_{Lu}}\right) u'(t - \Delta t) + \mu$$

where u'(t) is the turbulent velocity fluctuation at time *t*;
T_{Lu} is the Lagrangian integrated timescale
μ is a random acceleration

The models then assume that the velocity at time t is correlated with that at time *t-Δt* with a Lagrangian correlation coefficient $R_u(\Delta t)$. This leads to;

$$u'(t) = R_u(\Delta t) u'(t - \Delta t) + \sigma_{u'} \sqrt{1 - R_u^2(\Delta t)}\, u''(t)$$

where *u''(t)* is a random variable with mean 0 and standard deviation 1.
σ_u is the standard deviation of the turbulent velocity component.

It is usually assumed that the correlation coefficient decays exponentially with time:

$$R_u(\Delta t) = \exp\left(-\frac{\Delta t}{T_{Lu}}\right)$$

Similar equations apply in the *y,z* dimensions.

The values of T_{Lu} and σ_u are estimated from the meteorological conditions using similarity theory.

The dispersion of pollutants from industrial stacks is often influenced substantially by the presence of large buildings. Most of the plume dispersion models include simple algorithms to take account approximately of the influence of buildings. Lagrangian particle dispersion models such as PPM are able to calculate dispersion around buildings if the airflow pattern around the buildings is known.

Gaseous and particulate pollutants in the atmosphere in contact with the ground are deposited on the ground. Many of the models are able to estimate the rate of dry deposition and to take account of the resulting depletion of the plume emission from a point source. Pollutants are also washed out of the plume by the influence of rain. Many of the dispersion models are able to estimate the rate of wet deposition and the resulting depletion of the plume.

Air quality standards and objectives are usually expressed in terms of some statistical representation of pollutant concentrations, typically over a year. In local scale modelling applications, it is therefore required to determine the long term average pollutant concentration, the maximum hourly or daily average concentration or the n^{th} highest hourly concentration. Most dispersion models have the facility to calculate these statistics.

The rate of chemical reaction in the atmosphere for most of the chemicals in the EPER database is relatively slow. For local-scale modelling, it is usually acceptable to ignore chemical reactions of the pollutants. It is relatively straightforward to take account of first order chemical reactions both in plume models and in the Lagrangian particle dispersion models. The models are also applicable where reactions are pseudo first order, for example where there is a large excess of oxidant in the atmosphere reacting with the emitted pollutant. The models are not in general applicable where there are second or third order reactions of the emitted pollutant with other substances in the atmosphere. The reaction of nitric oxide emitted from industrial sources with ozone in the atmosphere to form nitrogen dioxide and the opposing photo dissociation in sunlight of the nitrogen dioxide receive special consideration in some of the models.

Most of the models are able to treat multiple emission sources. The models simply sum the concentration fields calculated for each individual source for each set of meteorological conditions. (The superposition or linearity principle is applicable provided that the dispersion of pollutants may be represented by a homogeneous linear differential equation).

Plume dispersion models are generally limited by the assumption that meteorological conditions remain constant during the period from emission to arriving at the receptor. In practice, this assumption limits the model range to less than about 50 km. The Lagrangian particle dispersion models are not limited in this way. Plume dispersion models are also not applicable at low wind speeds, generally less than approximately 1 m s^{-1}.

Plume dispersion models calculate the concentration at each receptor location individually, without reference to a model grid. It is usually convenient to specify the receptors on a rectangular or polar grid in order to facilitate the preparation of concentration maps. The number of receptor points on the grid is limited by computational time: typically concentrations are calculated at up to 10 000 receptor points allowing model runs with one year's hourly meteorological data to be completed in times from a few minutes to a few hours.

Lagrangian particle dispersion models also calculate particle dispersion without reference to a computational grid. However, pollutant concentrations are then calculated on the basis of the number of particles within volume elements. The volume elements need to be sufficiently large to contain an adequate number of particles to calculate the pollutant concentration. Model runs generally make a compromise between model spatial grid resolution, the number of particles and the computational time. The DIPCOT model typically takes 5 hr of CPU time (on an HP-720) to simulate 24 real hours of dispersion over complex terrain using 24 000 particles for a 40 x 40 x 13 meteorological grid. The GRAL model has reported computation times ranging from several hours to months on a Personal Computer depending on the complexity of the application.

The main features of the models assessed are summarised in Table 5.

Model evaluation
Many of the dispersion models are available commercially. The ISCST and AERMOD models developed for the US EPA and the AUSTAL2000 model are freely available from the Internet. The availability of each of the models, adequacy of documentation and applications history is indicated in Table 5. Documentation and application history is assessed on the scale shown in Table 4.

Table 4 Assessment system

Assessment level	Availability of documentation	Application history
Level 1	Good	Well-established models used for regulatory or policy purposes in the EU
Level 2	Generally satisfactory	Less widely used or less extensively validated, but generally based on established scientific principles.
Level 3	Less satisfactory	Newly developed models, or models based on novel principles or have not been extensively validated.

Several of the local-scale air dispersion models are very well documented with full descriptions of the algorithms used, detailed user manuals and peer-reviewed validation studies (Level 1). The computer codes for the US EPA models AERMOD and ISCST and the AUSTAL2000 model are freely available from the Internet. For most of the other models the level of documentation is generally satisfactory with the model algorithms described in detail in peer-reviewed papers (Level 2). However, some of the required documentation may not be readily available: for example, there may be no user manual. A few of the models are in a relatively early stage of their development or have only recently been made more generally available (Level 3). Detailed used guides may not yet have been prepared or the models may not have been extensively peer-reviewed.

The application history for each of the models was also assessed on the three level scale. Some of the models are well-established and have been widely used for regulatory purposes in the European Union (Level 1). These models have been compared extensively with measured concentrations close to point sources of pollutant emissions and the results of the assessments presented in peer-reviewed papers. For example, the performance of the models has been compared with other models in the series of workshops on Harmonisation within Atmospheric Dispersion for Regulatory Purposes ([14]). Other models (Level 2) are less widely used or have not been so extensively validated than the Level 1 models but are generally based on well-established scientific principles and have had some model validation carried out, sufficient to provide confidence in their application. A few of the models are relatively newly developed, are based on novel principles or have not been extensively validated against measured pollutant concentrations near point sources (Level 3).

Application examples

Dispersion models are most often used to predict whether the emissions from an industrial plant will lead to exceedances of an air quality standard or objective. For example, Figure 2 shows the 99.9 percentile 15-minute average sulphur dioxide concentrations predicted using the ADMS dispersion model in the vicinity of a proposed incinerator and a sugar processing plant. The predicted concentrations were compared with the United Kingdom objective of 266 µg m^{-3} as the 99.9 percentile of 15 minute mean concentrations.

There are relatively few comprehensive data sets of concentration measurements close to industrial point sources. The results of model comparison studies have been presented for many dispersion models at a series of workshops held as part of the European initiative on modelling harmonisation ([14]). The US EPA models AERMOD and ISCST have been most extensively evaluated against concentration measurements ([15]). There are many criteria for assessing the performance of dispersion models against monitoring data. Generally the models perform well when compared a cross a range of installations. For example, the overall model evaluation results for AERMOD version 02222 for sites not influenced by building downwash can be summarized as follows. Taking one composite (geometric mean) ratio of predicted to observed 'robust highest concentration' value for short-term averages at each site, and also taking the annual average ratio at sites with year-long databases:

- 1.03 is the overall predicted-to-observed ratio for short-term averages (with a range among sites from 0.76 to 1.35);
- 0.73 is the overall predicted-to-observed ratio for annual averages (with a range among sites from 0.30 to 1.64).

([14]) Harmonisation within atmospheric dispersion modelling for regulatory purposes http://www.harmo.org/.

([15]) http://www.epa.gov/scram001/7thconf/aermod/eval.pdf.

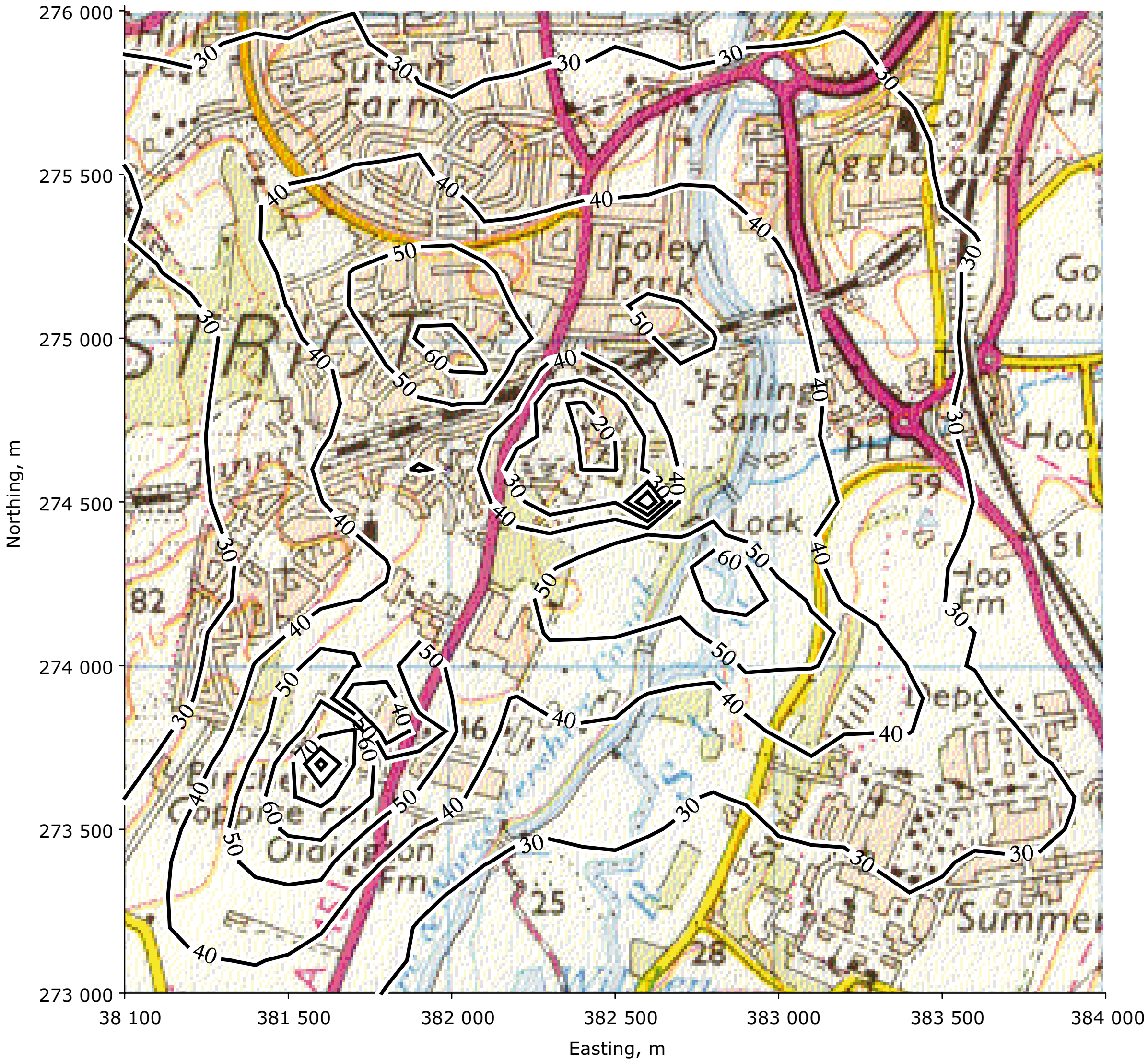
Table 5 Local-scale dispersion models evaluation

Model	Type	Availability	Plume rise	Complex terrain	Buildings	Deposition	Statistics	Chemistry	Multiple sources	Documentation	Validation history
ADMS	Plume	Commercial	√	√	√	√	√	NO_2	√	1	1
AERMOD	Plume	Internet/commercial	√	√	√	√	√	x	√	1	1
AEROPOL	Plume	From developer	√	x	√	√	√	x	√	2	2
AirQUIS-EPISODE	Plume	Commercial	√	x	x	√	√	NO_2	√	1	2
AUSTAL2000	Lagrangian	Internet		√		√		√	√	1	2
DIPCOT	Lagrangian	From developer	√	√	√	√	x	x	√	3	2
DISPERSION21	Plume	Commercial	√	x	√	x	√	x	√	1	3
EK100W	Plume	Commercial	√	x	x	√	√	x	√	3	2
GRAL	Lagrangian	From developer	√	√	√	x	x	x	√	2	2
HNS-TRANSMISSION	Plume	Commercial	√	x	x	√	√	√	√	1	2
IFDM	Plume	Commercial	√	x	x	√	√	x	√	1	1
INPUFF	Puff	From developer	√	x	x	√	√	x	√	2	2
ISCST	Plume	Internet/commercial	√	x	√	√	√	x	√	1	1
LASAT	Lagrangian	Commercial	x	√	√	√	√	√	√	1	2
MODIM	Plume	Commercial	√	x	x	√	√	x	√	2	3
NORMAL	Plume	From developer	x	x	x	√	√	x	x	1	2
OML	Plume	Commercial	√	√	√	x	√	x	√	2	2
OND-86	Plume	Commercial	√	√	√	√	√	x	√	1	1
ONM9440	Plume	Not available	√	√	x	√	√	x	√	2	2
PLUIM/PLUME Plus	Plume	Commercial	√	√	√	√	√	NO_2	√	2	2
POLGRAPH	Plume	Not available	√	√			√		√	3	2
PPM	Lagrangian	From developer				x		x		2	2
SPRAY	Lagrangian	Commercial	√	√		√		x	√	1	2
STACKS	Plume	Commercial	√	x	√					2	2
SYMOS-97	Plume	Commercial	√	√		√	√			2	3
ScalExNeuro	Plume	From developer	√	x	x	x	√	x	x	3	3
UDM-FMI	Plume	Not available	√	x	x	√	√	NO_2	√	3	3
VADIS	Lagrangian	From developer		x	√			x	√	3	3

Thus, the models are able to provide reasonable estimates of the maximum concentrations at an unspecified time and location near the installation. Over a period of time and over a variety of locations, the model predictions generally match the observations.

Scatter plots, which use data paired in time (and/or space), provide a more strict test, answering the question: 'At a given time and place, does the magnitude of the model prediction match the observation?' Generally scatter plots of this type show poor correlation between modelled and

Figure 2 **99.9 percentile 15 minute average sulphur dioxide concentrations, mg m^{-3}, from existing sugar processing and combined heat and power plant and proposed municipal solid waste incinerator**



Note: Based upon the Ordnance Survey 1:50 000 scale map with the permission of The Controller of Her Majesty' Stationary Office. © Crown Copyright. OS Licence AEA Technology Culham Abingdon Oxfordshire OX14 3ED AL51905A0001.

Maximum concentrations are shown at each location.

observed concentrations. The main limitation on the ability of dispersion models to predict concentrations at a specified time and place is the adequacy of data representing the wind field and turbulence structure of the atmosphere. Lagrangian particle dispersion models are able to make full use of detailed meteorological data or the results of computed wind and turbulence fields in complex terrain. Figure 3 shows a calibration plot of modelled and measured concentrations at rural, suburban and industrial monitoring sites.

Local-scale dispersion models are used to calculate pollutant concentrations in the vicinity of particular emission sources or groups of emission sources. Composite maps can be prepared of pollutant concentrations over wider areas. For example, Figure 4 shows modelled 99.73 percentile 1 hour average sulphur dioxide concentrations predicted for 2003 calculated using ADMS version 3.2 for the United Kingdom including all industrial sources with emissions greater than 500 tonnes per year of sulphur dioxide.

Figure 3 Calibration plot for 2003 99.73 percentile of 1-hour mean SO_2 concentrations

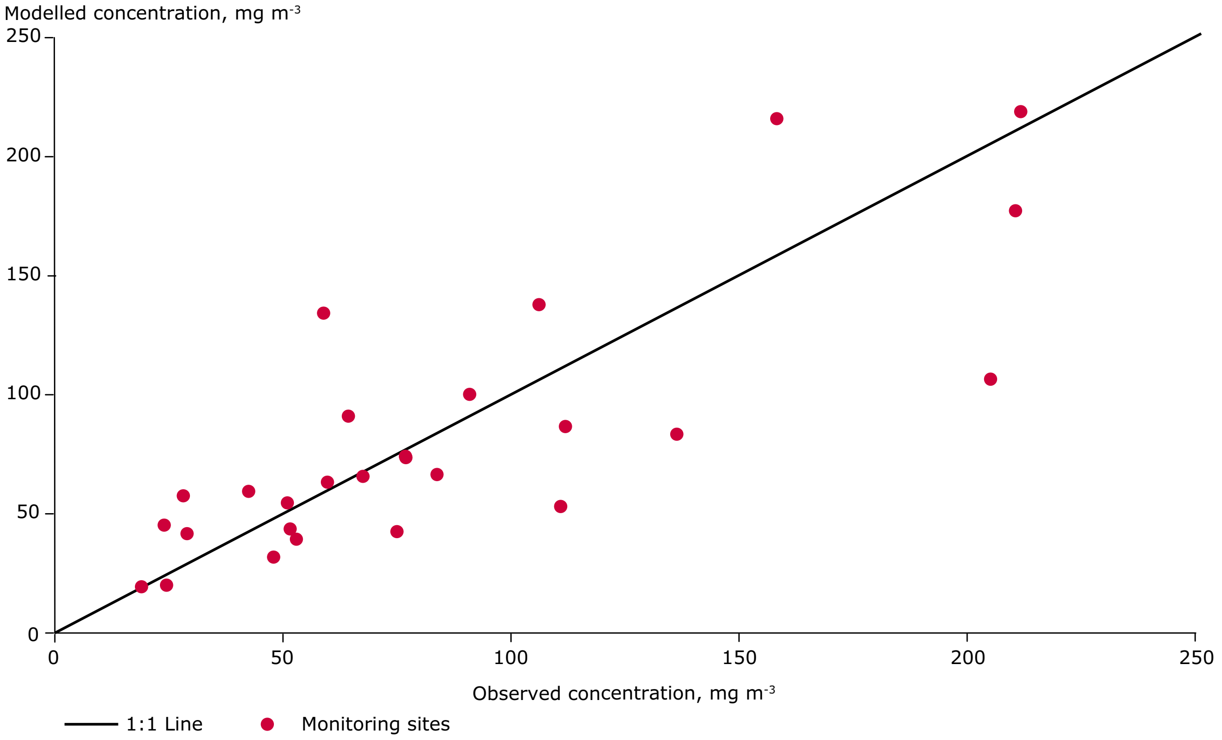
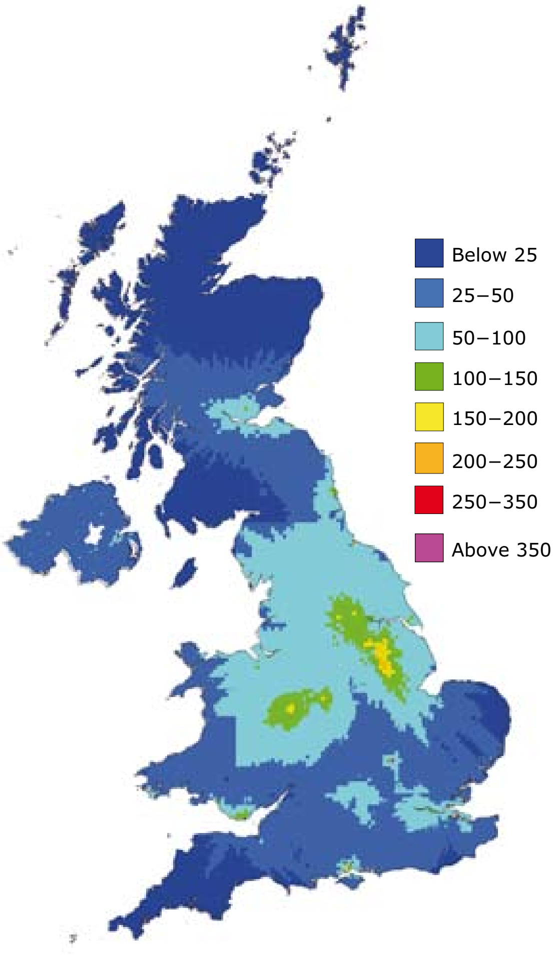


Figure 4 99.73 percentile of 1-hour mean SO_2 concentration, 2003 (mg m^{-3})



Model inputs
The following input data are usually required for local scale dispersion modelling:

Emissions data
Pollutant emission rates
Discharge height
Stack diameter
Discharge velocity
Discharge temperature

Meteorological data
Wind speed
Wind direction
Atmospheric stability data (e.g. cloud cover, surface heat flux, Monin-Obukhov length, Pasquill-Gifford stability category)
Boundary layer height
Friction velocity
Rainfall

Topography
Surface roughness
Terrain and building heights and coordinates

Deposition parameters
Dry deposition velocity
Washout coefficient

Receptors
Coordinates
Height above ground

Applicability of local dispersion models to EPER data
The local dispersion models discussed above are, in principle, applicable to any of the substances emitted to air as listed in EPER. However, it should be noted that of the above input data requirements, only total emissions to air per year for each installation, along with its geographical coordinates, are currently available in EPER. Local air dispersion models cannot therefore be used to generate accurate predictions of environmental concentrations from EPER data alone, without further input metadata on emission conditions, geographical, meteorological and other factors noted above. Given that the regulatory authorities commonly set emission permits on the basis of detailed modelling of environmental concentrations from emissions where these items of metadata are reasonably well characterised, it is important that such permitting decisions are not unnecessarily undermined through modelling in which inputs not available from EPER are estimated incorrectly, leading to erroneous results that may conflict with the regulatory analysis. In the absence of detailed metadata for highly spatially resolved dispersion modelling, it would appear preferable to use screening models that produce less highly resolved outputs based on standard metadata assumption, to generate 'reasonable worst case' estimates. Provided that model outputs are appropriately qualified as being based on the premise of reasonable worst-case conditions, then the potential for undermining of otherwise reasonable regulatory consents may be avoided.

Local dispersion models may, however, have application to predicting concentrations in air over a wider scale (hundreds of kilometres), for example, from multiple EPER sources as indicated in Figure 4. By taking a wider spatial scale, average meteorological data may be used, as at this scale the results are less sensitive to local features affecting dispersion. From consideration of the type of pollutant release and the nature of the releasing facility, it is often possible to make some informed estimates of the release conditions (e.g. stack height, continuous as opposed to batch releases etc.) that also impact on dispersion, in the absence of detailed information on these factors that is lacking in the EPER database.

3.2.2 Photochemical models

Photochemistry models are used to assess the contribution made to ozone concentrations resulting from the emissions of oxides of nitrogen and volatile organic compounds from anthropogenic sources, including the sources listed in the EPER database. Ozone is one of the strongest oxidising agents. It can lead to significant impairment of pulmonary function in humans, usually accompanied by respiratory and other symptoms. It damages the leaves of sensitive plants and affects photosynthesis. There are no significant emissions of ozone into the atmosphere. It is formed in the atmospheric boundary layer as the result of a series of complex chemical and photochemical reactions involving oxides of nitrogen and volatile organic compounds. Many other compounds and short-lived radicals are also formed as the result of these reactions. Photochemical models are also needed to predict the concentration of hydroxyl radicals in the atmosphere as these are usually the dominant oxidants that determine the persistence of organic chemicals released into the atmosphere. Some typical photochemical models are listed in Table 6.

Table 6 List of typical photochemistry models

Model	Information source
AirQUIS-EPISODE	http://www.nilu.no/airquis/models_episode_long.htm
CAMx	http://www.camx.com/overview.html
CHIMERE	http://euler.lmd.polytechnique.fr/chimere/V200501+/ShortDescription.html
EMEP Unified	http://www.emep.int/UniDoc/
EURAD	http://www.eurad.uni-koeln.de/index_e.html
EUROS	http://www2.dmu.dk/atmosphericenvironment/gloream/eurotrac2002/Glo11mensink.pdf
FARM	
LOTOS	http://homepages.cwi.nl/~gollum/LOTOS/
MARS	
MCCM	http://www.sma.df.gob.mx/modelacion/05/chapter5-nov.PDF
METPHOMOD	http://www.giub.unibe.ch/klimet/metphomod/
METRAS	http://www.mi.uni-hamburg.de/Mesoscale_Model_METRAS.359.0.html
MOGUNTIA	http://www.moguntia-global-modelling.de/
MUSE	http://www.ess.co.at/ECOSIM/forecasting.html
OFIS	http://aix.meng.auth.gr/saturn/annualrep01/other/OFIS_Abst.PDF
OPANA	http://atmosfera.lma.fi.upm.es/equal/equal/opana_doc.html
OSRM	http://atmos.chem.le.ac.uk/group/ppt/defra_031705.ppt
SMOG	
STOCHEM	http://www.metoffice.com/corporate/scitech0102/9_climate_research/atmospheric.html
TAPM	http://www.dar.csiro.au/tapm/
THOR	http://www2.dmu.dk/atmosphericenvironment/gloream/eurotrac2002/Glo03brandt.pdf
TNO-Isaksen	
TRANSCHIM	http://www.legi.hmg.inpg.fr/~Alpes/Internet/publications/brulfert/gratz_brulfert.pdf
TROPOS	http://www.odotech.qc.ca/troposimpact/tropos_impact_en.pdf
UK photochemical trajectory model	http://www.uea.ac.uk/~e044/apex/online.html

Modelling approaches

Photochemical models may be placed in two broad categories, as described for local air dispersion models, namely Eulerian and Lagrangian trajectory models.

Eulerian photochemistry models are based on the principle of mass conservation of pollutants. The models assume that the turbulent motion in the atmosphere can be resolved into a fluctuating component superimposed on the general mean flow. Similarly, fluctuations in concentration can be resolved into a fluctuating component superimposed on the general mean concentration. The mass conservation equation given in Box 4 then applies. Eulerian models are based on the numerical solution of the mass conservation equations for each of the chemical species at each node of a three-dimensional grid of receptor locations across the model domain. The models employ some form of turbulence closure to approximate the to the eddy flux terms. The simplest of these is the gradient transfer form, but more complex turbulence closure approximations are usually used in the vertical dimension. In some cases (e.g. the EMEP Unified model), dispersion in the horizontal plane is ignored.

The chemical and photochemical reactions in the atmosphere that lead to ozone production take place over several hundred or thousand kilometres. At this scale, the use of simple Cartesian coordinates may not be appropriate because of the shape of the earth. The equations are usually transformed to take account of alternative projections. For example, the EMEP unified model is transformed onto a polar-stereo graphic projection. Similarly, the models are usually transformed to take account of variations in terrain height.

A few of the models, mostly developed and applied in the United Kingdom, use the Lagrangian trajectory approach. This assumes that the pollutants are contained within a column of air which moves with the mean wind. Pollutants are emitted into the air column as it moves over each source. Chemical species are created or destroyed within the column of air or are removed from the column by wet or dry deposition.

The Lagrangian models used for the assessment of photochemical oxidant production assume that there is no dispersion of the pollutants in the horizontal plane. Many (e.g. OSRM, *UK photochemical trajectory model*) also assume that the pollutants are well-mixed throughout the atmospheric boundary layer, so that there is no vertical gradient in pollutant concentrations.

Photochemical models may also be categorized according to the scale of their model domains. Most of the models are designed to be used on the regional scale, typically covering the whole of Europe. Other models are used to predict photochemical oxidant concentrations over a global or hemispherical scale.

Model features

Photochemical models can be very demanding of computational resources. The models make a trade-off between the complexity of the scheme used to represent atmospheric chemistry, model resolution and computational time. Some of the models may attempt to model specific ozone episodes lasting a few days rather than simulate longer periods required for the calculation of ozone metrics for comparison with air quality standards.

The modelling domain used for photochemical studies typically includes the whole of Europe. Eulerian models have typically 100 grid points in each horizontal dimension and 10–20 grid points in the vertical dimension. The horizontal grid resolution is typically 50 km. Many of the Eulerian models have the capability to 'nest' grids so that the resolution can be increased in the main area of interest and decreased in more remote areas. Lagrangian models generally specify receptors locations on a regular Cartesian grid at typically 20 km resolution: the model domain may extend beyond the receptor grid.

The chemical and photochemical reactions that produce ozone and other photochemical oxidants in the atmosphere are extremely complex, involving large numbers of compounds, intermediates and radicals. Photochemical models limit the number of species and chemical and photochemical reactions in order to control the computational resources required for practical calculations. Generally reactions schemes that deal explicitly with larger numbers of species and chemical and photochemical reactions might be expected to provide a more realistic simulation of the chemical reactions in the atmosphere at the expense of increase computation time. Table 7 summarises the numbers of chemical species and chemical and photochemical reactions included in some of the most widely used reaction schemes.

The Eulerian models represent the model domain as a three-dimensional grid of computational nodes. Increasing the number of nodes increases the capability of the model to resolve localised effects at the expense of computation time. The EMEP model covering Europe and the Atlantic approaches has a 132 x 11 grid, 20 layers deep: A typical model run covering one year requires 11 real time hours (352 CPU hours) on 32 MIPS R14000 1200 Mflops processors. The EUROS model with 52 x 55 x 4 layers uses the CBM IV chemistry scheme and takes 18 hours on a PC to calculate one year's data. Many of the models have the facility to nest higher resolution grids covering a small area within a larger coarser grid.

Photochemistry models are required to predict short-term variations in ozone concentration, because ozone has potential acute effects on human health and the environment. The models therefore require detailed meteorological data for the whole of the model domain at relatively high temporal resolution (typically 3-hourly of 6-hourly) at several heights. These data may be provided by Numerical Prediction Models such as HIRLAM or MM5. The models include modules to handle the interface with the meteorological data.

Model evaluation

The outcome of model evaluation is summarised in Table 8. The evaluation scoring system is the same as was used for the local air pollution models (Table 4).

Several of the models are freely available from the Internet, namely CMAQ/Models 3, CHIMERE, CAMx and METPHOMOD. The TAPM model is available commercially. The remaining models may be obtainable from the developers.

Photochemistry models are generally reasonably well documented. Detailed descriptions are provided for most of the models assessed in peer reviewed literature. CMAQ/Models 3 is particularly well-documented with detailed descriptions of all modules, user manuals, and source code all freely available on the Internet. The computer codes for CMAQ/Models 3, CHIMERE and METPHOMOD are freely available from the Internet. For most of the other models the level of documentation is generally

Table 7 Examples of level of detail in air chemistry treatment in some widely-used photochemical models

Reaction scheme	Number of species	Number of chemical reactions	Number of photochemical reactions
CBM IV	36	93	11
RADM2	57	158	21
STOCHEM	69	142	15
EMEP	71	123	22
GRS	13	8	2

Table 8 Photochemistry models evaluation

Model	Availability	Type	Chemistry	Meteorology	Documentation	Application history
AirQUIS-EPISODE	Contact developer	Eulerian	Simplified EMEP	MATHEW	1	2
CAMx	Internet	Eulerian	Various	Various	1	2
CHIMERE	Internet	Eulerian	Simplified EMEP	MM5	1	2
CMAQ/MODELS3	Internet	Eulerian	Several detailed schemes available	MM5 3-D field	1	2
EMEP Unified	Not yet	Eulerian	EMEP	PARLAM-PS	2	2
EURAD	Contact developer	Eulerian	Various	MM5	1	2
EUROS	Limited	Eulerian		HIRLAM	2	2
FARM	Contact developer	Eulerian	Various	Various	2	2
LOTOS		Eulerian	CBMIV	NMI	2	2
MARS	Contact developer	Eulerian	Various		1	3
MCCM	Contact developer	Eulerian	RADM2	MM5	1	2
METPHOMOD	Internet	Eulerian			1	2
METRAS	Contact developer	Eulerian	Various		1	2
MOGUNTIA	Contact developer	Eulerian, global	Various		2	3
MUSE	Contact developer	Eulerian	Various		2	2
OFIS	Contact developer	Eulerian	EMEP		3	3
OPANA	Contact developer	Eulerian	Various		2	2
OSRM	No	Lagrangian	Various	UK Met Office	2	2
SMOG	Contact developer	Lagrangian			3	3
STOCHEM	No	Lagrangian, global	Stochem	UK Met Office	2	2
TAPM	Commercial	Eulerian	Simple generic	Australian Bureau Met	1	2
THOR	Contact developer	Eulerian, hemisphere		MM5	2	2
TNO-Isaksen	No	Eulerian, global			3	3
TRANSCHIM	No	Eulerian	Melchior	Various	3	3
TROPOS	Contact developer	Eulerian		UK Met Office	3	2
UK photochemical trajectory model	Contact developer	Lagrangian	Various	UK Met Office	2	2

satisfactory (Level 2) with the model algorithms described in detail in peer-reviewed papers. However, some of the required documentation may not be readily available: for example, there may be no user manual. A few of the models are in a relatively early stage of their development or have only recently been made more generally available (Level 3). Detailed used guides may not yet have been prepared or the models may not have been extensively peer-reviewed.

Most of the models have been developed for the purposes of national or regional policy development: thus CHIMERE has been used extensively in France, EURAD and METRAS have been used extensively in Germany, LOTOS in the Netherlands, EUROS in Belgium, OPANA in Spain, METPHOMOD in Switzerland and OSRM and the *UK photochemical trajectory model* in the United Kingdom. Recently, the performance of several of the photochemical models was compared as part of the City Delta European modelling exercise in support of the EU CAFE programme ([16]).

Model inputs
The following input data is generally required for models used to assess the production of photochemical oxidants in the atmosphere. Inputs shown in italics may not be required in simpler models.

Emissions data
Pollutant emission rates
Time dependence of emission rates
Discharge height
Stack diameter
Discharge velocity
Discharge temperature

Meteorological data
Wind speed *(at various heights throughout the atmospheric boundary layer)*
Wind direction *(at various heights throughout the atmospheric boundary layer)*
Atmospheric pressure and temperature
Atmospheric stability data (e.g. cloud cover, surface heat flux, Monin-Obukhov length)
Cloud cover, cloud water concentrations, relative humidity
Boundary layer height
Friction velocity
Rainfall

Background concentrations
Global/hemispherical background concentrations of oxidants, free radical species, etc.

Topography
Surface roughness
Terrain height details
Land cover types

Deposition parameters
Dry deposition velocities for each species
Washout coefficients for each species
Surface ozone flux parameterisation for deposition to vegetation (phenology, temperature dependence, light dependence, soil moisture content dependence, humidity dependence)

Chemistry
Details of reaction scheme
Chemical and photochemical rate constants

Receptors
Coordinates

Applicability of photochemistry models to EPER data
Photochemistry models may be applied to relevant releases listed in EPER (i.e. VOCs, oxides of nitrogen) and other sources of these chemicals, such as vehicle exhausts and natural VOCs released from vegetation. Because of the highly episodic nature of photochemical oxidant formation, a high level of detail on meteorological conditions is required, along with information on the timing of releases. This latter information is not available in EPER so therefore modelling would depend on best estimates to determine the impact of reasonable worst-case releases.

Many of the EPER sources make substantial contributions to oxides of nitrogen and VOC concentrations. They may therefore have a substantial effect on oxidant concentrations throughout Europe. Use of the EPER database with photochemistry models would allow the contribution to oxidant concentrations associated with regulated point sources to be assessed. The assessment would assist policy development relating to further regulation of EPER sources.

Many of the pollutants contained in the EPER database react with species formed in the atmosphere by photolysis such as the hydroxyl radical and ozone. It is often convenient to model the degradation of these compounds in the atmosphere by assuming that concentrations of the

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[16] http://rea.ei.jrc.it/netshare/thunis/citydelta/

oxidants are unaffected by the pollutant release so that it is possible to define an oxidant concentration field *a priori*. However, this simple approach may be in error where an EPER substance is released simultaneously with large quantities of oxides of nitrogen and VOCs. The use of the EPER database with a photochemical oxidant model to predict local oxidant concentrations would provide a more realistic prediction of atmospheric degradation rates.

3.2.3 Acid deposition and eutrophication models

Sulphur dioxide and oxides of nitrogen emitted from industrial point sources such as power stations, oil refineries and steel works make a substantial contribution to acidifying pollution. These gases are oxidised in the atmosphere to sulphuric and nitric acids respectively. The gaseous sulphur dioxide is transformed to particulate sulphate while nitric acid may be present as a gas or within particles or cloud droplets. The pollutants are removed from the atmosphere by dry deposition at the ground or are washed out by snow or rain. Over time this deposition ('acid rain') has resulted in the acidification of acid sensitive soils and water bodies to the detriment of associated vegetation and wildlife. Livestock production units are major sources of ammonia. The ammonia reacts in the atmosphere with sulphuric acid and nitric acid to form aerosol particles that deposit and contribute to the acidification of the soil and water bodies. The deposited nitrogen derived both from the ammonia and from the oxides of nitrogen contributes to eutrophication. The aerosol particles also contribute substantially to particulate matter concentrations (PM_{10}, $PM_{2.5}$) in the atmosphere.

Several specialised models have been developed to investigate the contribution made by industrial and other sources to acidification and eutrophication. These models have been used historically in the development of the National Emissions Ceiling Directive and the Gothenburg Protocol. Several typical models are listed in Table 9.

Several acid deposition models (e.g. TRACK, FRAME and WTM) have been used to model the deposition of inert substances such as heavy metals bound to particulate matter. The parts of the models used to predict chemical reaction rates are not used in this application.

Modelling approaches

Like local air dispersion and photochemical models, acid deposition and eutrophication models may be placed into two broad categories: Eulerian and Lagrangian models. The principles of these contrasting approaches have been described in the section on local air quality models, above.

The chemical reactions in the atmosphere that lead to acidification take place over several hundred or thousand kilometres. As with other large scale models, the use of simple Cartesian coordinates may not be appropriate because of the shape of the earth. The equations are usually transformed to take account of alternative projections. For example, the EMEP unified model is transformed onto a polar-stereo graphic projection. Similarly, the models are usually transformed to take account of variations in terrain height. Detailed modelling using the Eulerian models can require extensive use of powerful computing resources. Source-receptor matrix models

Table 9 List of typical models for acid deposition and eutrophication

Model	Information source
ADEPT	http://www.cefic.be/lri/Templates/shwProject.asp?NID=42&HID=419&S=35&PID=101
CHIMERE	http://euler.lmd.polytechnique.fr/chimere/V200501+/ShortDescription.html
CMAQ/MODELS3	http://www.cmascenter.org/html/model_doc.html
EMEP Unified Model	http://www.emep.int/index_model.html
EURAD	http://www.uni-koeln.de/math-nat-fak/geomet/eurad/index_e.html
HARM	http://www.cosis.net/abstracts/EAE03/09534/EAE03-J-09534.pdf
HILATAR	http://www.fmi.fi/research_air/air_25.html
IMSM	http://www.chmi.cz/uoco/isko/ptl/finiv.html
FRAME	http://www.frame.ceh.ac.uk/description.htm
LADM	http://www.emep.int/index_model.html
LOTOS	http://homepages.cwi.nl/~gollum/LOTOS/
RAINS	http://www.iiasa.ac.at/rains/Rains-online.html?sb=8
TAPM	http://www.dar.csiro.au/tapm/
TRACK	
WTM	http://www.externe.info/

such as RAINS and ADEPT have been developed to allow the results of the more complex models to be applied more generally. Source-receptor matrices are calculated on the basis of a set of given meteorological conditions that are used to estimate the contribution of an emission taking place in any one grid point to the development of concentrations or depositions in all of the grid points. In other words, each receptor square receives input from itself plus every other point in the matrix. It is therefore reasonably straightforward to calculate the impact of any one or more sources on concentrations or deposition experienced in the receptor matrix. This approach allows the chemical concentrations to be calculated without having to run the highly complex and time-consuming meteorological model each time.

Several of the models use the Lagrangian trajectory approach. As for the photochemical models, Lagrangian acidification and eutrophication models are based on the assumption that the pollutants are contained within a column of air which moves with the mean wind. Pollutants are emitted into the air column as it moves over each source. Chemical species are created or destroyed within the column of air or are removed from the column by wet or dry deposition. The Lagrangian models used for the assessment of acidification and eutrophication assume that there is no dispersion of the pollutants in the horizontal plane. Many (e.g. WTM, HARM) also assume that the pollutants are well-mixed throughout the atmospheric boundary layer, so that there is no vertical gradient in pollutant concentrations.

Acidification and eutrophication are relatively slow processes. The models are therefore only required to predict long-term average rates of deposition. It is therefore typical of Lagrangian trajectory acidification models to use statistically-averaged meteorological data. For example, WTM and TRACK calculate rates of deposition at each receptor along 24 trajectories at 15º intervals and assign a frequency weighting to each trajectory based on a statistical analysis of meteorological data.

Model features

Sulphur dioxide and oxides of nitrogen emitted from industrial point sources undergo a limited range of chemical reactions. Some of the most important reactions are listed in Table 10. In the past, models have considered a limited range of chemical species directly involved in the oxidation and deposition of the sulphur and nitrogen leading to acidification and eutrophication. These models have assumed that the oxidants (ozone, hydroxyl radical, hydrogen peroxide, etc.) are present in the atmosphere at some background concentration and that the oxidants consumed by reaction are replenished. More recently, increased computing power has allowed 'one atmosphere' models to be used (e.g. CMAQ/Models 3) in which the production and destruction of oxidants in the atmosphere is modelled directly. The models are then required to calculate the concentrations of many chemical species (typically 70): the resulting computational times can be rather long. A wide range of alternative chemical schemes of varying complexity is used in modelling acidification.

The modelling domain used for acidification and eutrophication studies typically includes the whole of Europe. Eulerian models have typically 100 grid points in each horizontal dimension and 10–20 grid points in the vertical dimension. The horizontal grid resolution is typically 50 km. Many of the Eulerian models have the capability 'nest' grids so that the resolution can be increased in the main area of interest and decreased in more remote areas. Lagrangian models generally specify receptors locations on a regular Cartesian grid at typically 20 km resolution: the model domain may extend beyond the receptor grid.

The Eulerian models require detailed meteorological data for the whole of the model domain at relatively high temporal resolution (typically 3-hourly of 6-hourly) at several heights. These data may be provided by Numerical Prediction Models such as HIRLAM or MM5. The Eulerian models include modules to handle the interface with the meteorological data.

Model evaluation

The results of model evaluation are summarised in Table 11. Few of the acidification models are available commercially, although CMAQ/Models 3 and WTM are freely available from the Internet. The scoring for evaluation uses the same system developed for local air quality models.

Acidification and eutrophication models are reasonably generally well documented. Detailed descriptions are provided for most of the models assessed in peer reviewed literature. CMAQ/Models 3 is particularly well-documented with detailed descriptions of all modules, user manuals, and source code all freely available on the Internet.

None of the acid deposition and eutrophication models is judged to be sufficiently well-established and to have been widely used for regulatory purposes in the European Union (Level 1): generally

Table 10 Key reactions contributing to acid deposition

Process	Chemical equation
Oxidation of nitric oxide by ozone	$NO + O_3 \rightarrow NO_2 + O_2$
Photodissociation of nitrogen dioxide	$NO_2 + hv \rightarrow NO + O_3$
Oxidation of nitrogen dioxide by hydroxyl radicals	$OH + NO_2 + M \rightarrow HNO_3 + M$
Oxidation of nitrogen dioxide by ozone	$NO_2 + O_3 \rightarrow NO_3 + O_2$
Photodissociation of NO_3	$NO_3 + hv \rightarrow NO_2 + O_3$
Reaction of nitric acid with ammonia	$NH_3 + HNO_3 \rightarrow NH_4NO_3$
Reaction of nitric acid aerosol species	$HNO_3 \rightarrow$ aerosol
Production of dinitrogen pentoxide	$NO_3 + NO_2 \rightarrow N_2O_5$
Reaction of N_2O_5 with aerosol species	$N_2O_5 \rightarrow$ aerosol
Gas phase oxidation of sulphur dioxide by the hydroxyl radical	$SO_2+OH \rightarrow H_2SO_4$ (gas phase reaction)
Aqueous phase oxidation of sulphur dioxide by hydrogen peroxide	$SO_2+H_2O_2 \rightarrow H_2SO_4$
Aqueous phase oxidation of sulphur dioxide by ozone	$SO_2+O_3 \rightarrow H_2SO_4$
Reaction of sulphuric acid with ammonia	$2NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4$

Table 11 Acid deposition and eutrophication models

Model	Type	Chemistry	Grid nesting (Eulerian only)	Meteorological data	Availability	Levels of documen-tation	Application history
CMAQ/ MODELS3	Eulerian	Several detailed schemes available	Yes	MM5 3-D field	Internet	1	2
EMEP Unified Model	Eulerian	UNI-ACID/ UNI-OZONE	No	PARLAM-PS 3-D field	Not available	2	2
EURAD	Eulerian	RADM2	Yes	MM5 3-D field	Contact developer	2	2
HARM	Lagrangian	Acid precursors only		Statistical	Not available	2	2
HILATAR	Eulerian	Limited chemistry	No	HIRLAM	Contact developer	2	2
IMSM	Eulerian	Limited chemistry	No		Contact developer	3	2
FRAME	Lagrangian	Acid precursors only		Statistical	Not available	2	2
LADM	Lagrangian	Acid precursors only			Not available	2	2
LOTOS	Eulerian	Modified CBM-IV	No	NMI Numerical Weather Prediction	Contact developer	2	2
RAINS	Source-receptor based on EMEP unified model	No		None	Internet	2	2
TAPM	Eulerian		Yes	CSIRO	Commercial	1	2
TRACK	Lagrangian	Acid precursors only		Statistical	Not available	2	2
WTM	Lagrangian	Acid precursors only		Statistical	Contact developer	2	3

models have been developed to assist national or regional policy development and have not been adopted widely outside their countries of origin. However, most are based on well-established scientific principles and have had some model validation carried out, sufficient to provide confidence in their application (Level 2). A few of the models are relatively newly developed, are based on novel principles or have not been extensively validated against measured pollutant concentrations near point sources (Level 3).

Model inputs
The following input data is generally required for models used to assess acidification and eutrophication impacts. Inputs shown in italics may not be required in simpler models.

Emissions data
Pollutant emission rates
Discharge height
Stack diameter
Discharge velocity
Discharge temperature

Meteorological data
Wind speed *(at various heights throughout the atmospheric boundary layer)*
Wind direction *(at various heights throughout the atmospheric boundary layer)*
Atmospheric stability data (e.g. cloud cover, surface heat flux, Monin-Obukhov length, Pasquill-Gifford stability category)
Boundary layer height
Friction velocity
Rainfall

Background concentrations
Global/hemispherical background concentrations of oxidants, free radical species, etc.

Topography
Surface roughness
Terrain height details
Land cover types

Deposition parameters
Dry deposition velocities for each species
Washout coefficients for each species

Chemistry
Details of reaction scheme
Chemical and photochemical rate constants

Receptors
Coordinates

Applicability of acidification and eutrophication models to EPER data
The greatest numbers of releases reported in the EPER database are for ammonia and oxides of nitrogen. Substantial numbers of releases of sulphur oxides are also reported in the EPER database. It is therefore likely that EPER emission sources make a significant contribution to acidification and eutrophication and also to secondary particulate concentrations in the atmosphere. The acidification and eutrophication models provide useful tools for assessing the contribution of EPER emissions to acidification, eutrophication and secondary particulate matter concentrations. The selection of acidification and eutrophication models is being considered in other work by the EEA: these models will therefore not be considered further in this study.

3.3 Multimedia models

Multimedia models have been developed to estimate fate and behaviour of a chemical in the environment on a large (regional or global) scale. They give an idea of the mass balance of a chemical and identify the environmental compartment(s) in which it tends to partition. They have been introduced for evaluative purposes. They do not exactly represent the real world but rather a simplified environment, which may help to improve understanding of the fate and behaviour of a substance. Depending on their level of sophistication, they may also give an indication of the relative importance of the various transfer and transformation processes and can contribute to an estimation of the distribution of a chemical between environmental compartments.

Multimedia models have particular application to assessing and managing the risks from chemicals that are persistent in the environment and have a potential for long-range transport. Such chemicals are known as POPs (persistent organic pollutants) and PBTs (persistent, bioaccumulating and toxic). Multimedia models can calculate the persistence of such chemicals and the potential for long-range transport (LRTP). They consider multiple environmental compartments, including air, water, sediment, soil and in some cases biota. Sophisticated multimedia models are used to track the movement of persistent chemicals in the environment, taking account of releases, atmospheric transport, deposition and resuspension and degradative processes. Because of the persistence and environmental mobility of some of these types of chemicals, an important consideration is the mobilisation of reserves of chemicals built up in reservoirs such as soils and sediments that may continue to recharge the atmosphere for years after the primary releases, and so contribute to pollution on a global scale. One of the major uses of multimedia modelling has therefore been in developing understanding of long-range transboundary movement of pollutants to assist policymaking in this area. Much of this work is being undertaken under the protocols on POPs and heavy metals within the framework of the UNECE Convention on Long-range Transboundary Air Pollution (CLRTAP) ([2], p.10).

3.3.1 Types of multimedia model

There is a wide range of multimedia models available, ranging from simple screening models to highly complex simulation models. Screening models are generally useful for ranking chemicals with regard to persistence and LRTP, rather than for making detailed predictions about environmental concentrations. Generally speaking, accuracy of a model increases up to a certain point with the number of processes that it attempts to simulate, which in turn requires more detailed data and input parameters. However, beyond a certain point increasing complexity of models does not result in greater accuracy of the outputs, because of the inherent uncertainty in the ever-more detailed inputs required. The OECD guidance document on the use of multimedia models (17) notes that there may be an optimum spatial resolution for a multimedia model, but points out that it is difficult to know where this optimum lies and its position will depend on the question to be answered.

Multi-media models assume a 'unit world' which is supposed to represent the actual environment on a large scale. This unit world is divided in several compartments with specified volumes. Most models consider six compartments: air, water, soil, sediment, suspended solids and aquatic biota, but this may vary. Each compartment is homogenous.

Once the unit world is defined, the models take into account different phenomena that may affect the fate of the chemical. Each of these phenomena is quantified and the set of equations obtained, together with a description of the discharge, constitutes the structure of the model.

Four levels of sophistication of multimedia models are generally recognised and these are summarised in Table 12. In progressing from Level I to Level IV, the fidelity of the calculations in simulating the 'real' world increases, but at the expense of greater requirements for input data describing both the chemical in question and the various environmental media involved in the analysis.

In addition to the four-level classification referred to above, models may also be classed according to how they reflect the environmental properties. Generic multimedia models do not attempt to simulate specific environments but instead use default values for typical environments. This allows them to be used for studying the impacts of chemical properties independently of the characteristics of particular environments. They are useful for determining how partitioning properties and degradability of the chemical determine transport and fate.

Region-specific models have been developed from generic models by parameterising environmental characteristics to reflect particular regions, usually by means of a geographical database. Region-specific models may include additional environmental compartments (such as groundwater, sediments, vegetation, etc.) or subdivide existing compartments — e.g. surface and sub-soil, multiple layers in the atmosphere, and so on). Obviously additional mass transfer and partition coefficients are also required with this additional level of complexity. An advantage of region-specific models over generic or evaluative models is that results can be directly compared with reported concentrations of contaminants in a specific area.

Multi-zone models provide a further level of sophistication. Multi-zone models consist of a series of regional models that are interconnected by advective fluxes of water and air. This approach has been used at both the global and more local scale of resolution. The intention is to increase accuracy by making the models more reflective of the actual geography of the region(s) studied. Such models have been used to predict the environmental fate and transport of POPs, in particular how alternating deposition and re-suspension can lead to a net movement of POPs from tropical and temperate zones to cold regions.

Highly detailed outputs of spatially-disaggregated concentrations in a wide range of environmental compartments, varying in time to allow long-term trends to be estimated, are produced by complex transport and fate models based on general circulation models. Examples of these models include EMEP, Hysplit4 and MCI-MCTM. The

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([17]) OECD (2004). Guidance document on the use of multimedia models for estimating overall environmental persistence and long-range transport. OECD series on testing and assessment No 45. 18 March 2004. http://appli1.oecd.org/olis/2004doc.nsf/linkto/env-jm-mono(2004)5.

Table 12 Complexity of multimedia models

Level	Key assumptions	Information obtained	Comments
Level I	Equilibrium partitioning Steady state Closed system	General partitioning tendencies for persistent chemicals	Screening type models for rapid assessment of the environmental media into which a chemical is likely to partition. Because Level I models do not take account of degradation, but instead rely on mass balancing by equilibrium partitioning alone, they cannot be used to calculate persistence and LRTP.
Level II	Equilibrium partitioning Steady state (Could be extended to dynamic) Open system	Estimate of overall persistence Important compartments for removal processes Relative importance of advection and degradation as removal pathways	These models include removal mechanism due to chemical transformations (biotic and biotic) and advection at the system boundaries, but retain the assumption of equilibrium partitioning among the environmental compartments. 'Level II dyn' (dynamic) models consider explicitly the time course of mass in all media. They are the simplest models to calculate persistence and LRTP
Level III	Non-equilibrium Steady state Open system	Influence of mode of emission on fate and transport Refined assessment of overall persistence and loss pathways	These models include the rates of inter-media transport. Mass balance conditions are applied to each environmental compartment. Although there is no requirement for equilibrium partitioning between adjacent, it is still assumed that chemicals achieve equilibrium among the available phases within a compartment.
Level IV	Non-equilibrium Dynamic Open system	Influence of mode of emission on P_{ov} and LRTP Time course of response of contaminant inventory by compartment to any time-varying conditions	Removal rates and rates of inter-media transport between environmental compartments are used to define a time-dependent description of mass distribution. The rate of chemical input to each compartment can be continuous or time-varying. This makes assessment of transient effects possible, such as seasonal variations in emissions and/or climate and soil conditions.

Note: Adapted from OECD Technical Guidance document ([17]).

models consider geophysical transport in the atmosphere and oceans on a global scale. They include a detailed treatment of atmospheric processes and include detailed meteorological data on wind speed, temperature and precipitation at various locations and altitudes. Models include approaches based on both Eulerian and Lagrangian dispersion methodologies, which are outlined in Section 3.2.1. Multi-zone models may include further spatial resolution by linking several region-specific models together to represent a continental or global scale.

3.3.2 *Data requirements for multimedia models*

Multimedia models require input data related to the properties and behaviour of the chemical under consideration, the environment into which it is released and the means of release. These factors are discussed below.

Chemical properties

Depending on the type of model, input data are needed to define the chemical of interest, the environment(s) receiving the substance and the mode of entry. Taking the nature of inputs relating to the chemical itself first, the main properties of interest governing the distribution between environmental phases (e.g. air-water, air-aerosols, air-soil, etc.) are partitioning coefficients and rates of degradation in relevant environmental phases.

Data on partitioning coefficients that govern the distribution of a chemical between environmental phases are available for many chemicals from measurements undertaken under standard conditions and reported in the literature and in extensive chemical databases. However, experimentally determined values may not be reliable, especially where values are very small — e.g. for substances with very low vapour pressure or low water solubility. The alternative to experimentally determined data is to predict partition coefficients from quantitative structure property relationships (QSPRs), for which numerous established models are available. The EC's Technical Guidance documents provide information on the use of QSPRs for chemical risk assessment ([18]). It should be noted, however, that the model results might be insensitive to values that lie outside a particular range. Special considerations are required when the substance in question ionises. In this case, the ionised specie(s) are assumed to be completely non-volatile and not to sorb to solids. Ionisation may be corrected for by using the non-dissociated fraction, calculated from the dissociation constant and the environmental pH. Further uncertainty in partitioning coefficient values comes from temperature dependence. Partitioning coefficients are determined under standard temperature and pressure, but these may differ significantly from temperature and pressure in the environment. Some multimedia models make the appropriate corrections, but it is up to the user to verify whether this is the case, or whether data corrected to environmental temperature and pressure has to be provided as a model input.

All models (other than Level 1) require data on degradation rates of chemicals in the various environmental media. As for partitioning coefficients, these data may be measured or derived from QSPRs. Some simplification of input data may be possible, since only those environmental compartments that contain significant amounts of the chemical may require an accurate degradation rate. The OECD guidance document reports that for compartments containing less than 5 % of the chemical a rough estimate of decomposition rate is usually acceptable. Extensive guidance is provided through the OECD ([17], p.39) on the use and selection of degradation data. Temperature dependence of reaction rates is an important consideration and generally speaking degradation rates should be corrected to the appropriate environmental temperature, using the Arrhenius equation.

Specific considerations affect degradation rates in various environmental compartments. For degradation in air, the dominant degradation reaction is through photo-oxidation with hydroxyl radicals, although direct photolysis is also important for substances with the correct absorption spectrum. Other oxidants (e.g. ozone and nitrate radicals) may also be important for particular types of chemical. A further complication comes with low vapour pressure substances that tend to sorb to aerosol particles. It is usually assumed conservatively that hydroxyl radicals do not degrade sorbed substances, but this assumption needs to be tested. Experimental data for decomposition rates in air are available for many substances and QSPRs may be used to derive them where experimental data are missing.

Degradation processes in water are dominated by hydrolysis, photolysis and biodegradation and the overall rate is taken as the sum of these processes. Rates should either be determined using published standardised procedures such as those given by OECD or alternatively they may be calculated from QSPRs. Similar mechanisms apply in soils and sediments, although of course photo-degradation is invariably restricted to surface layers (or possible to sediments suspended in the water column). Biodegradation is the dominant route for most non-polar organics, but other processes may also be important for other classes of chemical. The availability of degradation rate data is generally less than for air and water, although it is reasonably well covered for pesticides. Degradation rates vary with soil conditions — organic matter and clay mineral content, pH and water status and these factors too should be taken into account. Similarly degradation data for sediments tends to be even scarcer than for soils. This shortage of data has led to the adoption of simple multipliers to estimate half-lives of chemicals in sediment from corresponding soil or water data. The current EU approach assumes that sediment half-lives may be approximated as 10 times the soil half-life. Leaching of chemicals from surface soil into deeper layers or into groundwater should also be considered.

Some models include consideration of decomposition of chemicals in vegetation also. Chemicals may be filtered from the gas phase by plant canopies. The chemicals may then be degraded in/on the plant tissue (by metabolic or photolytic processes) or may be transported to the ground after leaf fall. Very few data are available on decomposition rates in vegetation and further work is needed to provide this information, particularly for low volatility substances (such as POPs) where vegetation is an important component of the system.

It is important to remember that models do not necessarily account for all of the processes

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([18]) European Commission. 2003. Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances, and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market.

that influence chemical mobility. For example, partitioning between water and air, particularly for non-polar organic substances, is influenced by more processes than are included in most models, including such poorly characterised factors like soil texture and condition, plant species and physiology.

Environmental properties
Turning now to the environmental data needs of multimedia models, this will include information on:

- Meteorological data — wind speed, direction, air temperature, depth of mixing layer;
- Hydrological data — annual (or other time period) rainfall, runoff, infiltration, ground water recharge, surface water depth, sediment loads;
- Soil properties — bulk density, porosity, water content, erosion rates and root zone depth.

Generic models usually provide default environmental data, but location-specific models will require this information to be provided. GIS datasets are now available characterising wide areas of Europe (and elsewhere) for input data, which are described later.

Release details
Finally, the remaining class of data required for multimedia models defines the release of the chemical to the environment — whether it is to air, water or soil. For chemical risk assessment generally, it is important to consider all routes of entry to the environment throughout the life of the product (i.e. from manufacture, use and disposal, etc.). Relevant information on release routes from particular uses of a chemical is given in Emission Scenario Documents. Examples are given in the EU Technical Guidance documents ([18], p.41). Other sources of data include the OECD Emission Scenario Documents and individual country emission scenario documents provided via OECD, OECD and national compendia of PRTR release estimation techniques. Where only releases from an industrial point source need to be considered, as in the present feasibility study, the requirement for release data is obviously limited to this single route. However, a number of factors that affect the dispersion of a chemical following its release will also need to be considered, such as release height, plume buoyancy, continuous or batch release, and so on.

3.3.3 Multimedia models for screening purposes

A number of generic multimedia models were identified that are suitable for predicting environmental concentrations of chemicals resulting from point source emissions but which do not produce spatially or temporally resolved outputs. These models have largely been developed for screening or evaluative purposes, mostly on a regional scale. The models are listed in Table 14.

Model evaluation
All of the models listed in Table 14 are multimedia Level I, II, III or IV fugacity type models, except for RiskPoll, which is a uniform world model. In all cases, the underlying concepts and examples of usage of the models has been reported in the peer-reviewed literature, and information about the models is in all cases judged to be sufficient for users to make use of the models. In most cases, the software and documentation are available for free download from the Internet. We have not identified web site for downloading ChemFrance and SimpleBox models. In the latter case, however, the model forms the basis of the EUSES (described below), which is itself available as a free web download. All of these generic models run on standard PCs under the Microsoft Windows® operating system. They all produce output that can be stored as spreadsheets, CSV or other formats.

The models have been developed for a range of specific purposes and applications. For example, CoZMo-POP (coastal zone model for persistent pollutants, a Level IV model) ([19]) was developed specifically to study the long-term fate of POPs in a coastal environment or large lake basin, in particular to distinguish between atmospheric and soil sources of POPs over a long period. It is a simplified version of the POPCYCLING-Baltic model (described below). The current version of the model (CoZMo-POP 2), released in 2005, builds on the first version which came out in August 2000. The model would appear to offer a good solution for its target application but appears to be less suited for screening point source emissions of POPs for environmental distribution outside these types of environment.

The EQC (Equilibrium Criterion) model has been designed for preliminary screening of chemicals to establish the media into which they will tend to partition, loss mechanisms and tendency for

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([19]) Frank Wania, Knut Breivik, N. Johan Persson and Michael S. McLachlan (2005). CoZMo-POP 2 — A fugacity-based dynamic multi-compartmental mass balance model of the fate of persistent organic pollutants. Environmental Modelling and Software — in press.

inter-media transport. It offers the choice of Level I, II or III fugacity modelling approaches and can be used for a wide range of chemicals. The characteristics of the environment (based on notional regions) are fixed within the model.

ChemCAN is a rather more complex spatially-resolved screening model based on Level III principles. It comes with 24 regions representing parts of Canada already defined as the default regions, but these could be replaced with European regional data for use in this continent, providing the regions are not less than 300 km radius. ChemCAN predicts average concentrations of chemicals in air, water, fish, sediments, vegetation and coastal waters. It was developed to assist human exposure to chemicals calculation. ChemFrance is a similar model developed for France, in which the country is divided into 12 regions (plus a further region considered as the entire country).

A couple of models have been developed specifically to calculate persistence and potential for long-range transport, using Level II or III principles. The ELPOS (Environmental Long-range Transport and Persistence of Organic Substances) model is based on the regional part of SimpleBox/EUSES. It comes with a chemical database of 100 current use pesticides and POPs and allows the user to calculate the overall persistence and characteristic travel distance. The version of the model currently available on the Internet is version 1.0.1, dated September 2001, suggesting that the model is not still under development. An alternative tool is the TaPL3 model, which works as a Level II fugacity model, which may be useful for evaluative screening for potential for long-range transport, particularly in comparing results for different chemicals. The developers recommend that a Level III model (which will take account of advection between media) be used for 'absolute' assessments of chemicals. TaPL3 allows releases to either air or water as the mobile medium to be evaluated. The current version is v3.00, dating from September 2003.

EUSES is the most widely accepted tool for use in the EU for predicting the environmental concentrations of new and existing chemicals. EUSES is a decision support model based on Level III fugacity principals that can be used to undertake risk assessments, in accordance with the detailed technical guidance provided by the European Commission ([18], p.40). The essence of the approach set out in the technical guidance documents is that the predicted concentration of the chemical in question is calculated and then compared with an estimated no-effect level for a variety of human health and environmental endpoints. The greater the ratio between the no effect level and the predicted concentration, the greater is the confidence that releases of the chemical will not cause adverse effects. EUSES is available for PC users for free download from the European Chemicals Bureau web site. The current version is 2.0.3.

Application of screening models to EPER emission sources

Several of the models discussed above could be suitable for predicting environmental concentrations at local, regional and continental scale of chemicals released from industrial sources, such as those listed in EPER. However, EUSES would appear to have a number of advantages for such application, given that it has been designed specifically to fulfil the requirements of the EC Technical Guidance Documents on chemical risk assessment, it has been extensively peer-reviewed and is the widely-accepted tool in the EU for chemical risk assessment. This stands it in good stead to be used for the related application of assessing concentrations from point-source releases.

The EU technical guidance methodology enshrined in EUSES considers releases of chemicals from all stages of its life cycle. These may differ appreciably depending on the use pattern of the chemical — and default values for proportion released are provided for different emission scenarios. The user may over-write these defaults with more realistic data as this becomes available, in order to progressively improve the reliability of EUSES output. In order to estimate environmental concentrations arising from a point source emission, EUSES would need to have all releases associated with the manufacturing stage.

EUSES adopts a nested approach for calculating concentrations in the regional and local scale. Local concentrations are assumed to derive from the local release plus background concentrations derived from all other sources in the region, other than the one under consideration. Regional concentrations in turn are based on regional releases plus a background concentration in air or water flowing in from the surrounding continent. Table 13 illustrates the inputs and outputs of EUSES.

Local estimates of environmental concentration are applied to point source emissions and relate to a standard hypothetical environment and the concentrations experienced within the border of the facility making the emission. In the case of concentrations in air, this would relate to a point 100 meters from the emission source. For deposition

Table 13 EUSES model inputs and outputs

Inputs required	Outputs
Physico-chemical properties Characterisation of the environment Emission data Partitioning coefficients Degradation rates Fate in sewage treatment plants Physico-chemical properties Characterisation of the environment Emission data Partitioning coefficients Degradation rates Fate in sewage treatment plants	**Local PECs**
	Microorganisms in STP Surface water (dissolved) • during an episode • annual average Sediment (total) Air (total) — annual average Agricultural soil (total) • averaged over 30 days • averaged over 180 days Grassland (total) • averaged over 180 days Porewater in agricultural soil Porewater in grassland soil Groundwater under agricultural soil
	Regional PECs
	Surface water (dissolved) Air (total) Agricultural soil Natural soil Porewater of agricultural soil Sediment (total)

to soil, an area of radius 1 000 meters around the source is considered. A number of default assumptions are made concerning the nature of the release and the characteristics of the receiving environment that ensure that the calculated local concentrations are 'reasonable worst case'. These take account of the dilution and dispersion of the chemical in the receiving medium (air or water), rates of reaction and deposition (from air), adsorption by sediment (water) etc. The default values for the relevant parameters in EUSES may be substituted by more appropriate data where this is available, or reasonable assumption based on the nature of the process under consideration. For example, if the source were a large power station stack, then a discharge height of (say) 100 meters would be more reasonable than 10 meters. This would usually have the effect of reducing the predicted environmental concentration in the locality, in effect moving from a reasonable worst case to a reasonable average case basis. For example, in the case of emissions to air, releases are assumed to take place at a height of 10 meters, with no plume rise. In practice, many point source releases will take place from chimneys at least 100 meters tall, and with considerable plume buoyancy. Taking these factors into consideration where the data are available will lead to a much more realistic estimate of local air concentration at ground level compared with the reasonable worst-case assumption.

In calculating regional environmental concentrations, the technical guidance ([18], p.40) foresees two alternative approaches. The first is based on a standardised hypothetical region with agreed model parameters. The second uses country-specific model parameters. The technical guidance recommends that the first approach should be used, as a first approach for risk assessment and then the second approach adopted as more information is available on location of emission sites. In estimating regional concentrations resulting from point source emissions, a similar approach may be worth following, with initial calculations made using the hypothetical standardised region and then, where better geographical data are available, to make the calculation with region-specific data. This would enable users to explore the impact of site location of a facility releasing a certain chemical impacts on the predicted environmental concentrations. It would, however, result in different predicted concentrations from the same emission, depending on the characteristics used for different regions, which may make comparison at the EU level difficult.

Continental scale predicted environmental concentrations are calculated from releases in the EU plus Norway. These form the background concentrations used by the regional model. For persistent compounds, a further tier in the form of hemispheric or global background concentration may also be appropriate as the background or the continental scale. The nested approach requires that continental concentrations be first calculated as the background to regional levels, which in turn then form the background for local concentration estimation.

In principle, EUSES can be applied to any chemical and therefore could be applied to any of the substances listed in EPER. However, certain chemicals change their properties very markedly depending on environmental conditions. Generally speaking, the fugacity approach holds most strongly for non-polar, non-ionising organic substances. For other substances, the phase partitioning may be markedly affected by the environmental pH. This should therefore be taken into account in providing input data to on chemical properties, as described in (for example) by OECD. Heavy metals are particularly problematic, given that they may exist in a wide variety of forms in environmental media with widely differing bio-availabilities and toxicities. Furthermore, metals are naturally present in the environment and significant natural background levels may be found in soils, sediments and natural waters. With the exception of mercury, most metals generally do not have a significant volatile form. When emitted to the atmosphere, these other metals exist in the aerosol fraction and so can be modelled according to the movement and deposition of aerosol particles generally. Certain metals may change greatly in terms of bioavailability, depending on environmental properties, such as pH, redox potential and the presence or absence of other substances such as sulphide, with which they may form highly insoluble complexes. The EU technical guidance documents provide further information relevant to how metals should be treated for risk assessment. It should be noted in this context that models which calculate mass balances based on concentrations or masses of chemicals, as opposed to fugacity, have the advantage of being better suited to modelling involatile substances, without having to make specific adjustments such as the so-called 'aquivalence' approach (20) (21). Because models driven by air/water and solids/water partition coefficients (like EUSES, SimpleBox and ELPOS), rather than by vapour pressures, solubilities and octanol-water partition coefficients (like many of the other multimedia fate models, often referred to as fugacity models), they allow modelling of non-hydrophobic chemicals (e.g. metals) for which intermedia partitioning cannot be easily predicted from the elementary physical-chemical properties.

The final model (RiskPoll (22)) listed in Table 14 differs from the fugacity models in that it is based on the uniform world approach. RiskPoll is a set of simplified risk assessment tools for quantifying impacts on public health, agriculture and materials from the routine release of chemicals. The model can currently assess the damage costs of air pollution associated with respiratory disease associated with nitrogen oxides, sulphur dioxide, particulate matter, carbon monoxide and secondary aerosols, impacts of sulphur dioxide on agricultural crops and materials. In a multimedia mode, it can also assess the damage costs of heavy metal releases. The model, which is available as a spreadsheet, is transparent, easy to use and requires very little input data. The uniform world approach is based on the assumption of a source-based coordinate system, a steady emission rate, uniform population distribution, uniform depletion rate of airborne pollutants (through deposition plus degradation) and linear dose-response relationships. The damage costs are calculated from the predicted concentration and the damage cost per unit concentration for each impact. RiskPoll is coded in Microsoft Visual Basic 6.0® and is available for download (23) for use on a standard Windows-based PC. Microsoft Excel v7® or later and Adobe Acrobat® are also required.

3.3.4 *Spatially resolved models*

A selection of spatially resolved multimedia models is listed in Table 15. The table also includes a number of large scale atmospheric models that have been applied to regional, continental and hemispheric scale modelling of chemical transport. They include models based on both Eulerian and Lagrangian atmospheric dispersion methodologies. The table lists models that may be worth further consideration as possible tools for predicting environmental concentrations from EPER data. In general, for the purposes of tracking environmental concentrations of chemicals due to particular point source releases, regional or possibly continental scale modelling is of greatest relevance. Models that operate on the global scale are more concerned with the long-term distribution resulting from repeated inter-media exchanges, in which releases (past and present) from

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(20) Diamond, M.; Mackay, D.; Welbourn, P.M. (1992). Models of multimedia partitioning of multi-species chemicals: The fugacity/aquivalence approach. Chemosphere 25:1907–1921.

(21) Mackay, D.; di Guardo, A.; Paterson, S.; Cowan, E. (1996). Evaluating the environmental fate of a variety of types of chemicals using the EQC model. Environmental toxicology and chemistry 15:1627–1637.

(22) RiskPoll: a model for estimating public health and environmental impacts of air pollution. Spadaro, JV (2004). http://www.arirabl.com/software/RiskPoll %20Overview.pdf.

(23) For down loading RiskPoll, go to: http://www.arirabl.com/software.htm.

Table 14 Multimedia models for screening and evaluation

Model	Type	Outputs	Landscape	Applications	Availability	Levels of documentation	Application history
CoZMo-POP 2	Level IV	Average concentrations in air, fresh surface water, soils, vegetation, fish and marine coastal water.	Up to 19 compartments, including the forest, soils and fresh water bodies of the drainage basin, and a variable number of sequentially arranged marine water units.	Modelling the long-term fate of POPs in a coastal environment or the drainage basin of a large lake.	Free download	2	3
Chem-Can	Level III	Average concentrations in air, fresh surface water, soils, vegetation, fish and marine coastal water.	Supplied with regions representing 24 Canadian regions. User can define alternatives (min 300 km radius)	Generic chemical fate assessment.	Free download	2	2
Chem-FRANCE	Level III	Steady state concentrations in air, water, soil and vegetation.	Regional modelling of 12 regions of France and France itself.	Generic chemical fate assessment.	Contact developer	3	2
Simple-Box	Level III	Steady state concentrations in air, water, soil and vegetation.	Default regional, continental and global environments that can be customised by user.	Generic chemical fate assessment. SimpleBox has been incorporated into EUSES.	Contact developer	2	2
EQC	Levels I, II and III	Steady state concentrations in air, water, sediment and soil.	Fixed environments defined as defaults. Cannot be varied by user.	Evaluative — especially for chemical to chemical comparison	Free download	2	3
ELPOS	Level II or III	Steady state concentrations in air, water, sediment and soil. Persistence and characteristic travel distances.	Regional — based on regional part of EUSES — SimpleBox.	Assessment of persistence and characteristic travel distance for persistent organic compounds	Free download	2	2
TaPL3	Level II	Steady state concentrations in air, water, sediment and soil. Persistence and characteristic travel distances.	Fixed environments defined as defaults. Cannot be varied by user.	Evaluation of long-range transport and persistence for chemical to chemical comparison. Lack of advection means that it is unsuitable for absolute assessments.	Free download	2	3
EUSES	Level III	Average concentrations in air, surface water, soil, sediment.	Nested calculation based on continental, regional and local areas. The user may define regional characteristic.	Risk assessment of new and existing chemicals in compliance with EU Technical Guidance Documents.	Free download	1	1
RiskPoll	Uniform World Model	Average concentrations in air, water, soil, crops and associated damage costs.	Uniform	Screening for impact costs of classic air pollutant, heavy metals and POPs	Free download	2	2

regions are of greater relevance than those from particular point sources. Global models and models not covering the European continent have therefore been ruled out from further evaluation. These models are as follows:

CliMºChem: Global multi-compartment box model which does not have spatial resolution in the E-W direction (24).

ChemRange: Spatially homogeneous one dimensional circular system ('loop') global model (25).

GlobPOP: A global model that considers the world as 10 climatic zones (26).

MEDIA: Research model for studying the global distribution of HCH (27).

BETR: Based on the ChemCan Level III fugacity model, this model has been specifically developed for North America. (A European model based on BETR, known as EVN-BETR, is available).

Several of the models listed in Table 15 are highly complex models requiring substantial computing resources to operate, with typical run times extending to several hours or even days. They cannot be run on PCs and are generally not available as downloads or commercial products. The Hysplit atmospheric model can be run on a PC with downloaded meteorological data or run interactively over the Internet. CMAQ — Models 3 (also an atmospheric model) requires Linux or Unix parallel processor workstations. The Impact 2002 model, available in a non-spatial form as an Excel® spreadsheet available through the Internet can be run on a standard PC platform.

The following sections illustrate the types of applications for spatially resolved models which predict the distribution of persistent organic compounds and heavy metals. They also consider the types of input data required for the models and give examples of outputs, using the EMEP multimedia POP and heavy metals models for illustration. Examples of other large scale models are then summarised, before discussing the outcome of several model inter-comparison studies.

EMEP models for POPs and heavy metals
Arguably the most widely-used multimedia model in the international policy arena is the EMEP model used for certain POPS and heavy metals modelling under the UNECE Convention on Long-range Transboundary Air Pollution. The model, developed by Meteorological Synthesising Centre East (MSC-E) (28) , predicts the concentration and deposition of POPs and heavy metals from emissions within the EMEP grid for the following purposes:

- evaluation of atmospheric transport and deposition on regional (EMEP) scale;
- evaluation of spatial distribution in the atmosphere and soil, and for POPs, vegetation and sea water, too;
- evaluation of transboundary transport;
- evaluation of partitioning between main environmental compartments;
- assessment of temporal and spatial trends;
- projection of future levels of contamination and trends under various emission scenarios;
- estimation of long-range transport potential and overall persistence of new potential POPs;
- study of environment pollution on the basis of monitoring/modelling approach.

The pollutants currently modelled are (POPS): B(a)P. B(b)F, B(k)F, PCBs, PCDDs/PCDFs, gamma-HCH and HCB, and (heavy metals): lead, mercury and cadmium. A pilot parameterisation for arsenic, chromium and nickel is also under way. The model, which is under continuous development, is described in detail by MSC-E and the following discussion summarises key points from this source.

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(24) Wegmann, F. (2004). Thesis submitted for the degree of doctor of natural sciences, Swiss Federal Institute for Technology Zurich (ETHZ). Thesis number 15427. http://e-collection.ethbib.ethz.ch/ecol-pool/diss/abstracts/p15427.pdf.

(25) Chemrange 2.1 — A Multimedia Transport Model for Calculating Persistence and Spatial Range of Organic Chemicals M. Scheringer, H. Held, and M. Stroebe (2003). http://ltcmail.ethz.ch/hungerb/research/product/chemrange.html.

(26) Wania, F. and Mackay, D. (2000). The global distribution model: A non-steady state, mass balance model for the fate of persistent organic pollutants in the global environment. http://www.scar.utoronto.ca/ %7Ewania/reports/GloboPOP.pdf.

(27) Koziol A. and J. Pudykiewicz (2001): Global scale transport of persistent organic pollutants, Chemosphere, 45 (8), 1181–1200. http://www.cmc.ec.gc.ca/~arqidor/report_2000/html_files/report.html.

(28) MSC-(E) POP model description. http://www.emep.int/index_pollutants.html.

Table 15 Spatially resolved multimedia and large scale atmosphericmodels

Model	Scale	Resolution	Type	Chemicals	Availa-bility	Levels of documentation	Application history
EMEP	Regional (EMEP region) and hemispheric	Regional model 50 x 50 km grid. 150 x 150 km grid in hemispheric version	3-D Eulerian, multimedia.	Certain POPs, Pb, Cd and Hg	Not available	2	1
EVN-BETR	Continental — European	Europe is devided into 54 5 x 5 deg grids (i.e. about 300 x 300 km at 60 deg N)	3-D Eulerian multimedia	Certain POPs	Contact developer	3	3
G-CIEMS	Regional — Japan (can be parameterised for Europe)	Air: Grid cell: 5 km by 5 km for Japanese terrestrial area (about 40 000 grid cells) and 100 km by 80 km for oceanic area (about 7 000 grid cells) area. Surface water and soil. Total of 38 000 catchments, consisting of river path and catchment area.	Fugacity / mass balance multimedia	Certain POPs	Contact developer	2	2
MPI-MCTM	Global		Based on global circulation model. Multimedia	Certain POPs	Contact developer	3	3
IMPACT 2002	Regional	Soil and water based on 135 watersheds, air and ocean on 2 x 2.5 deg grids.	LCIA exposure model for calculating human intake fraction of a released chemical.	Organic and inorganic	Non-spatial version available as web download.	2	2
ADOM	Hemispheric	76 x 76 domain of 55 x 55 km grids, 12 layers up to 10 km.	3-D Eulerian atmospheric	Hg, certain POPs	Contact developer	2	2
DEHM	Hemispheric	150 x 150 km grid, nested to 50 x 50 and 16.75 x 16.75 km over Arctic	3-D Eulerian, atmospheric	Certain POPs, Pb, Hg	Contact developer	3	3
HYSPLIT 4	Any	Multiple resolution concentration output grids	Lagrangian atmospheric	Any	Web download (free of charge to approved users)	2	2
	Local to continental	Multiple scale	3-D Eulerian atmospheric	Any	Web download	2	2

The EMEP regional model is a three-dimensional Eulerian multi-compartment model operating within the geographical scope of the EMEP region on a 50 x 50 km grid. There is also a hemispheric model with a grid resolution of 2.5 x 2.5 degrees. The hemispheric model is used for calculations of transport and accumulation on hemispheric scale, for evaluation of pollution of the European region by remote sources, for evaluation of intercontinental transport, for assessing of pollution of remote regions like, for example, the Arctic region. The regional models consider the main environmental compartments (atmosphere, soil, sea water, vegetation) and include basic processes describing POP and heavy metal emissions, long-range transport, deposition, degradation, and gaseous exchange between the atmosphere and the underlying surface. The model domain covers practically the whole troposphere, upper layer of soil of 20 cm, and sea water compartment within the model grid.

Evaluation of pollution levels within the European region requires appropriate information on initial concentrations in the environmental compartments and influence of emission sources outside the model grid. Initial concentrations of POPs and heavy metals in the main environmental compartments are calculated in model runs using historical emissions of particular pollutants. For substances with significant long-range potential initial concentrations can be calculated using the hemispheric models. The influence of emission sources outside the model domain can be taken into account using measurement data or by the use of the hemispheric model. The lack of available monitoring data requires that the influence of remote emission sources is evaluated by means of the hemispheric model. For this purpose the hemispheric model is run with all hemispheric emissions, excluding sources within the EMEP grid. The contribution of European emission sources to the pollution levels within the EMEP grid is obtained by means of the regional EMEP POPs and heavy metal models.

Input data for the EMEP models
Detailed meteorological data are key input parameters for modelling long-range transport and deposition of atmospheric pollutants. The quality of the modelled concentrations and depositions is determined to a large extent by quality of the meteorological data. Modelling of POPs and heavy metals requires a large set of meteorological parameters, including:

- wind velocity components at different altitudes of the troposphere for modelling advection;
- three-dimensional precipitation rates for modelling wet removal processes;
- various atmospheric boundary parameters (e.g. friction velocity, Monin-Obukhov length etc.) for modelling dry deposition.

Most of the parameters are not available from routine meteorological observations. Moreover, observation stations are randomly distributed over the surface, whereas the model needs data on a regular grid. Therefore, it is necessary to use a preprocessing system, which can prepare gridded meteorological parameters with certain temporal resolution. The model is meant for utilizing off-line meteorological information. This means that meteorological data are not generated in the process of calculations, but periodically supplied into the model as input data. Therefore, meteorological data have to be prepared in advance and stored in the same model grid as used in the transport model. Direct interpolation of meteorological parameters to the model grid is not acceptable because it can significantly disturb the mass conservation. Besides, some parameters (e.g. atmospheric precipitation) cannot be correctly interpolated in principal. Hence, in order to provide the model with meteorological data a preprocessing system has been developed based on the PSU/NCAR mesoscale model MM5. The system utilizes input meteorological data with rough spatial and temporal resolution and performs short-term weather forecast for the transport model grid.

Emissions data
The MSC-E POPs and heavy metal models use gridded anthropogenic emissions databased both on national information officially submitted by the Parties to the Convention and expert estimates. For countries that have not submitted national data, a linear interpolation from previous years or expert judgement is used to generate the input data needed for the modelling.

The vertical distribution of the pollutant concentration in the vicinity of emission sources, as well as long-range atmospheric transport, depends on the height of the emission source. For example, emissions from road transport take place near surface, whereas stacks of power stations can be as high as 100 to 200 meters. Besides, thermal or dynamical effects can lead to significant lifting up the emissions in the atmosphere. In order to estimate distribution of emissions with height, MSC-E utilises sector-split emission information provided by 20 countries. Height distributions for different emission sectors are averaged taking into account a sector contribution to the total emission. Plume rise is not currently taken into account.

Anthropogenic emissions of heavy metals have a noticeable temporal cycle (daily, seasonal etc.). Production of heat and, hence, emissions from this sector results in emission increase in winter season. Emissions from the road transport sector and from electric power production are lowest at night. Seasonal variation of the emissions is taken into account in the model. The average seasonal emission amplitudes are calculated from multi-years emissions data. Seasonal emissions can vary not only from country to country, but also in different parts of a big country. However, at present these amplitudes are applied for the whole domain.

Physicochemical properties
Physicochemical properties of POPs and heavy metal emissions are also taken into account. Lead, cadmium and some other heavy metals (nickel, chromium, zinc etc.) and their compounds have very low volatility. Therefore, it is assumed that they are emitted to the atmosphere in aerosol particles. Mercury can be emitted both in gaseous and in particulate forms. Besides, gaseous species include elemental and oxidized forms. The speciation of mercury emissions is not usually included in the information submitted by the Parties to the Convention, so therefore this is based on expert judgement.

Similarly, emission data for modelling POPs is made on the basis of official submissions and expert judgement, including expert estimates of seasonal variation. The overall toxicity of PCDD/F mixture according to different congeners and spatial distributions of emissions for each congener are taken into account. Further details of how this is done are given by MSC-E ([28], p.47).

Basic differences in the long-range transport of POPs mainly result from peculiarities of their physicochemical properties and degradation rates in the main environmental media. The key characteristics required for POP modelling are the following:

- Sub-cooled liquid vapour pressure;
- air-water Henry's law constant;
- washout ratio for the particulate and gaseous phase;
- degradation rate constants for different environmental compartments;
- coefficients of partitioning between different media (octanol-water partition coefficient, octanol-air partition coefficient, organic carbon-water partition coefficient;
- data on the distribution of low volatile POPs with particle sizes in the atmosphere; and
- molecular diffusion coefficients.

Values for these parameters are obtained from the literature or from experimental measurements.

Landscape data
Land cover data is mostly required for evaluation of the dry deposition velocities and assessment of ecosystem-specific depositions. Currently a preliminary land cover dataset is used in the model. It has 17 land use/land cover categories including various types of forest, agricultural crops, water bodies, tundra and desert, ranging from boreal to Mediterranean conditions. The dataset is partly based on the database developed in the framework of EC Programme on Coordination of Information on the Environment (Corine ([29])). Since the Corine land cover data do not cover the entire EMEP area, Stockholm Environment Institute (SEI) database was used to fill the gaps ([30]). In order to unify the Corine and SEI inventories ecosystem classification EUNIS (European Nature Information System) was adopted. Parameterisation of dry deposition requires some characteristics of the ground surface depending on land cover category (roughness length, height of vegetation canopy, displacement heights). These characteristics vary from season to season. Five different seasonal categories are considered in the model.

In addition, for POPs modelling, which takes account of deposition to vegetation, the Leaf Area Index (LAI) data set is needed for the description of POP gaseous exchange between the atmosphere and vegetation. The Leaf Area Index for a given grid cell is the ratio between the area of leaves to its geographical area. The NASA Goddard Space Flight Center provided the geographically resolved leaf area index data with monthly resolution. Data on sea currents were obtained from ocean general circulation model (OGCM). These data describe the three-dimensional structure of velocity fields in the oceanic depth and the surface mixed layer depths within the EMEP grid. The velocity fields and the upper mixed layer thickness are defined for every two days with linear interpolation of values obtained within this period of time.

([29]) dataservice.eea.europa.eu.
([30]) http://www.york.ac.uk/inst/sei/APS/projects.html.

Examples of outputs from EMEP
Some examples of geographically resolved outputs from the regional EMEP models (31) for POPs and heavy metals are shown in Figure 5 and Figure 6 (below) which are taken from the EMEP website. Note the use of the polar stereo graphic projection and resolution given by the 50 x 50 km grid within the EMEP area. The examples demonstrate the value of the map-based output to locate apparent 'hot spots' of high emissions and depositions, and to resolve emissions into anthropogenic and natural sources. Figure 5 also shows trends in emissions and resulting loadings in air, sea water and soil. Figure 7 shows an example of output from the POPs hemispheric model for comparison, in this case for the pesticide gamma HCH (also known as 'Lindane'). Note the coarser scale needed to plot hot spots on a hemispheric scale.

In considering the EMEP output data, it is important to remember that the predicted geographical distributions are entirely based on computer modelling and have not been verified by measurements made on a comparable geographical and temporal basis. As with other models, the main driver for the predicted concentrations is the emission data: inaccuracies in this key input data will be reflected in the output obtained. Because of the scarcity of detailed input emission data for the EMEP source grid, expert judgement has been used to provide these inputs where better data are missing. These considerable uncertainties must therefore be taken into account when considering the reliability of the modelled concentrations obtained.

Not withstanding these limitations, EMEP provides additional detailed information on the contributions of the EMEP countries to POPs and heavy metal inputs over their own and other countries' territory. EMEP also provides similar information on acid deposition and eutrophication, and photochemical oxidants.

Other large scale multimedia and atmospheric models
Several other large-scale multimedia models are also available and have been used in a European context, along with some large-scale atmospheric models. Although these operate according to different principles (i.e. Eulerian, Lagrangian), the degree of complexity of the input data requirements is similar to that needed for the EMEP model. The models are briefly described below.

EVn-BETR
EVn-BETR is a fugacity-based, contaminant distribution model developed at Lancaster University with funding from the UK government (Department for the Environment, Food and Rural Affairs) in order to simulate the fate of POPs in the European Continent (32). The model calculates steady and non-steady state (dynamic) mass balances of chemical contaminants from inputs describing the environmental characteristics of Europe, the physicochemical properties of the chemical of interest, and contaminant emission rates. The focus is on describing pollutant fate and transport, including transfer, transport and cycling in and between air, vegetation, soil, surface water, sediments and coastal water. The European model builds on previous work carried out by the Canadian Environmental Modelling Centre and their North America (BETR) distribution model. Again, GIS software was used to better describe geo-referenced data regarding land cover, water flows, soil organic carbon content, precipitation and temperature information. The model divides Europe into 54 regions using a 5 x 5 degree grid. A total of 50 cells describe the main bulk of the European continent with four further perimetric boxes, namely: the Atlantic, Mediterranean, Eurasian and Arctic Boxes. There is also provision for a 55 region representing the world outside Europe. In this way, data extracted from various Global Circulation Models (e.g. ECMWF datasets) can easily be incorporated into the model. The model has been described in further detail by Prevadouros *et al.* (33).

G-CIEMS
Grid-Catchment Integrated Environmental Modelling System (G-CIEMS, tentative name) is a geo-referenced multimedia and river environmental fate model system for region-scale environment (34). Although developed for application in Japan, the model can be parameterised for Europe or other locations. The multimedia model is as an expansion of Mackay-type multimedia fate model to multi-box

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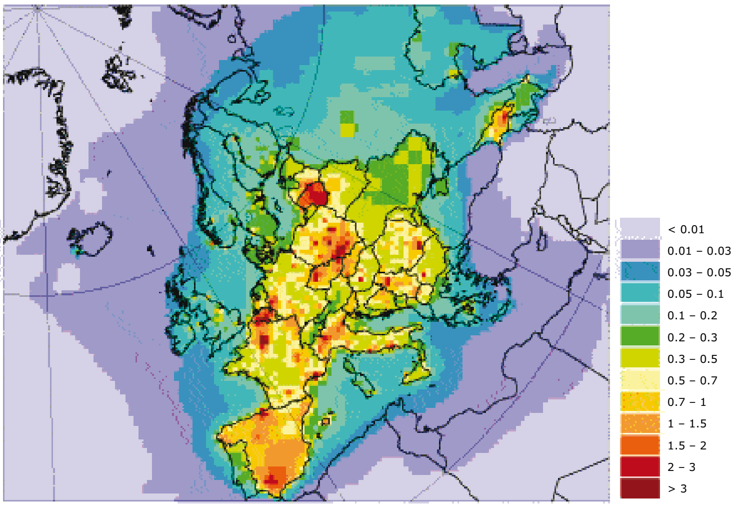
(31) See the MSC-E website for details of the figures shown here. http://www.msceast.org/.

(32) European Evn-BETR model, K Prevadousos. http://www.es.lancs.ac.uk/ecerg/kcjgroup/European_model.htm.

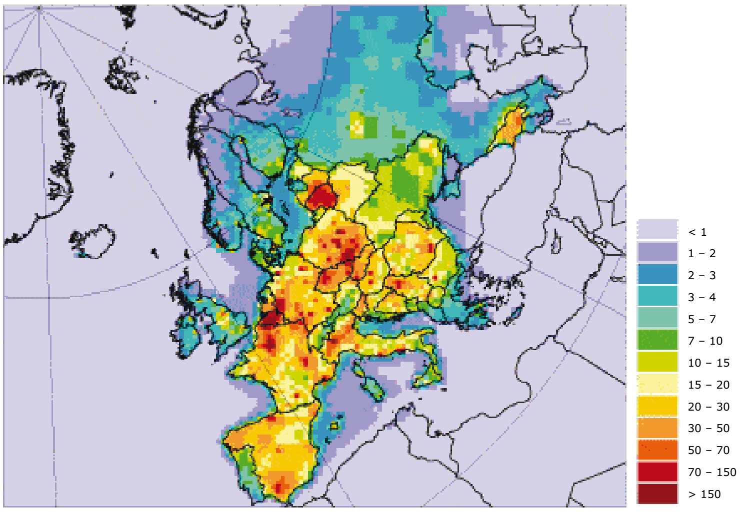
(33) Prevadouros, K. et al. (2001). Modelling the fate of persistent organic pollutants in Europe: Parameterisation of a gridded distribution model. *Environmental Pollution*, 128, 251–261.

(34) Suzuki, N. *et al.* (2004). Transport and fate characteristics of persistent organic chemicals around geo-referenced Japanese environment by spatially-resolved/geo-referenced model (G-CIEMS) methodology. Organohalogen Compounds, 66, 2392–2397. http://dioxin2004.abstract-management.de/pdf/p481.pdf.

Figure 5 Examples of EMEP regional POPs model output — Benzo(a)pyrene (B(a)P)



Mean annual B[a]P air concentrations in 2001, ng/m^3



Spatial distribution of B[a]P deposition in 2001, g/km^2/y

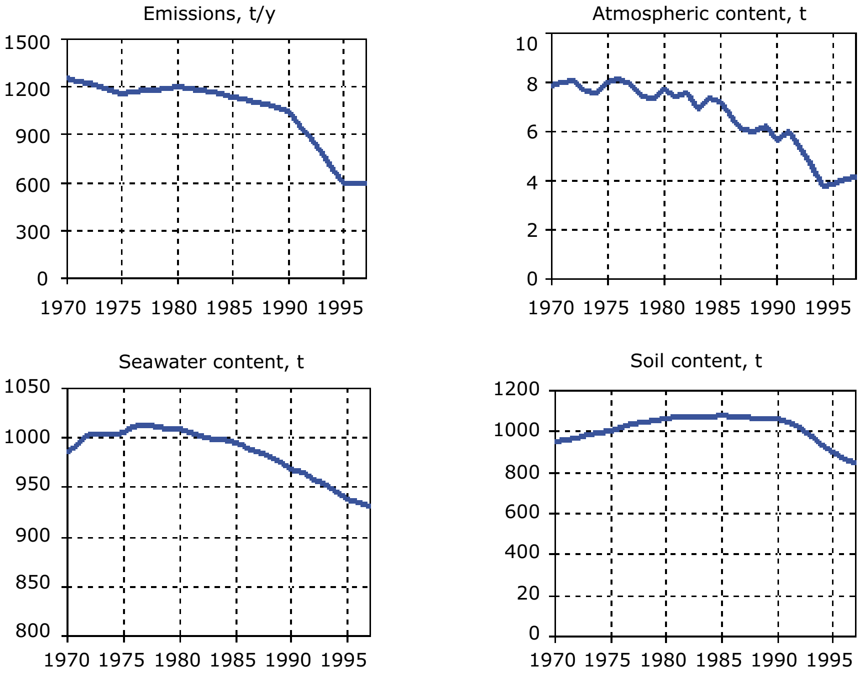
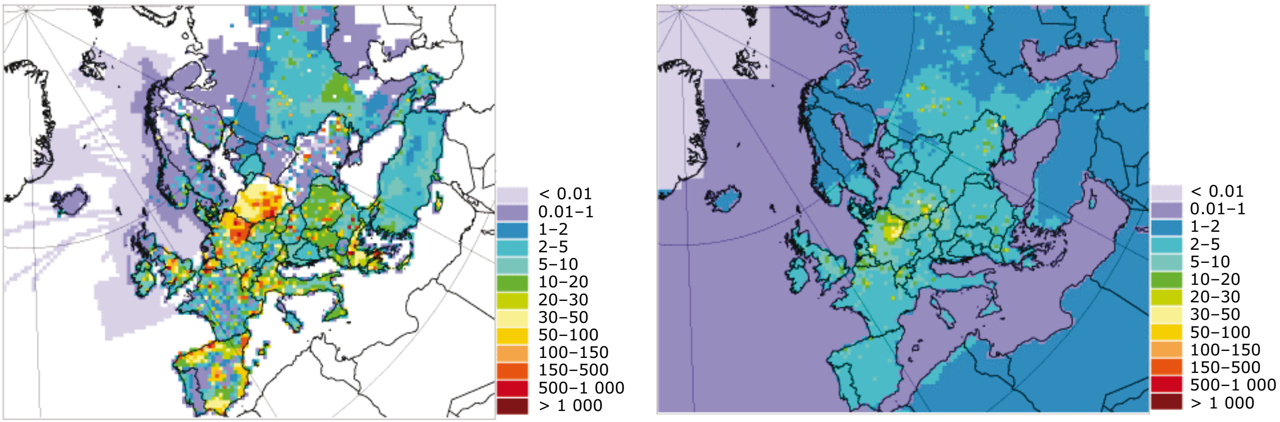
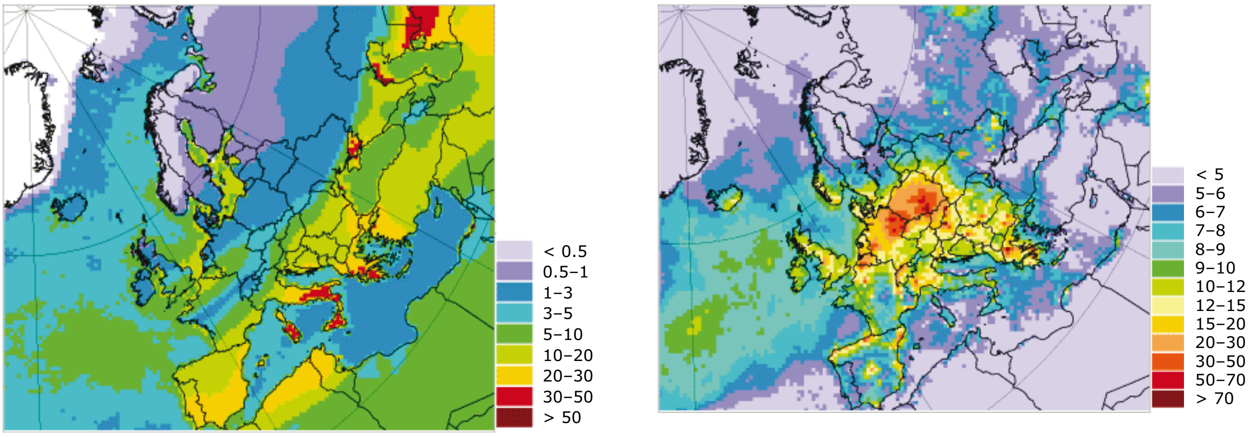


Figure 6 **Examples of EMEP regional heavy metal output — mercury emissions and deposition**



Spatial distribution of mercury anthropogenic emissions in 2002, g/km²/y

Mercury re-emissions field in the EMEP region with spatial resolution 50 x 50 km. a/km²/y



Spatial distribution of natural mercury emissions in the EMEP region, spatail resolution 50 x 50 km

Total (dry and wet) deposition of mercury in 2002, g/km²/y

compartments with geo-referenced geographical resolution on GIS software. The model calculates multimedia environmental concentration on specified geographical environmental area. The model consists of the following geographical/data items. Each item has relevant information like geographical/hydrological/meteorological and chemical datasets on database format. Air: grid structure with layers, now 5 x 5 km size. River: GIS line items representing real geographical river. Soil: GIS polygon items including seven land use categories and one forest vegetation compartment. Average size of soil polygon is around 10 km² at present. Lake: GIS polygon item, coastal area and coastal sea. Inter-media transport is formulated on diffusive and advective processes. The model is developed on a GIS-based integrated information system as the data management system and the user interface, based on Microsoft Access database. The model can calculate the gross POPs input and output between target area and outer boundary for each transport pathway.

MPI-MCTM

The MPI-MCTM (multi-compartment chemistry-transport model of the Max Planck Institute for Meteorology, Hamburg) is designed to describe the environmental fate of semi-volatile organic substances consistently with the geospheric transports and transformations including their geographic distribution and temporal variabilities. In the present state of model development it comprises atmosphere (three-dimensional), vegetation, soils and ocean (two-dimensional

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(35) Lammel, G., Feichter, J., Leip, A. (2001) Long-range transport and multimedia partitioning of semi volatile organic compounds: A case study on two modern agrochemicals. Max Planck Institute for Meteorology, Report No 324.

distribution of single layer boxes, each) (35). It is based on an atmospheric general circulation model (GCM). The surface properties (vegetation and soil type distributions, land and sea ice, soil hydrological status) and the large-scale atmospheric circulation patterns are well represented in GCMs. The atmosphere is a three phase system (gas, particles, cloud-water), with the mass exchange between them being controlled by instantaneous equilibria. Degradation is controlled by the hydroxyl and nitrate radical concentrations (three-dimensional fields varying with time of day and month). Wet and dry deposition processes are considered for various types. Deposition of the gaseous molecules to ground surfaces is described by fixed deposition velocities or by accounting for the atmospheric and surface resistances. The soil is a multiphase system. The ocean is a single phase (neglecting the hydrosol), two layer system (locally and seasonally varying depth of well-mixed surface layer). A three-dimensional ocean GCM will be coupled for the study of the environmental fate of substances, which in the long term, might accumulate in the ocean. The model accounts for first-order degradation processes in the compartments and volatilisation processes from the ground compartments into the atmosphere. The model is fully dynamic and can be run either in a climatological mode (then generating its own but realistic climate) or simulating historic climate (then driven by weather and sea surface observations).

IMPACT 2002

IMPACT 2002 is a multimedia multi-pathway exposure model for Western Europe (36). The model facilitates the estimation of environmental concentration distributions, related levels of contaminants in food and the fraction of a chemical release that will end up in the human population (the intake fraction) — an approach to modelling that has been successfully applied in the field of population risk assessment from the release of radioactive substances. Unlike the models discussed so far, IMPACT 2002 assesses human exposure as opposed to just estimating chemical concentrations in environmental media (37). The model exists in both spatial and non-spatial forms. The spatial form uses watershed boundaries for the soil and surface water compartments, based on 135 watersheds in the ERICA (European Rivers and Catchments) dataset (38) and 2 x 2.5 degree grid cells for air and ocean water. Annual food production rates were allocated to the watershed according the fraction of respective agricultural land coverage and information on population distribution, fish and drinking water extraction were derived from published sources and databases. An evaluation for disperse emissions of PeCDF (2, 3, 4, 7, 8-pentachlorodiphenyldioxin) showed reasonable agreement with monitoring data for most impact pathways in both versions of the model, although some improvement is needed in the vegetation models. The non-spatial version of the model appeared, on wider comparison with a range of diverse organic chemicals, to be adequate for assessing dispersed sources. However, in the case of point source emissions, models that are not spatially resolved can introduce errors (both under and overestimates) in population intake by at least 3 orders of magnitude for some chemicals. IMPACT 2002 can be used for organic and inorganic chemicals including metals. It is implemented as a Microsoft Excel® spreadsheet model and runs on standard PCs. The non-spatial version is available as a web download. IMPACT 2002 has been developed specifically for population-level assessments of chemical impacts on the human population via food, drinking water and inhalation. Unless this specific application is the desired aim of the modelling exercise, the model would appear to offer few advantages over established multimedia models, such as EUSES, for assessing environmental concentrations.

ADOM

The comprehensive atmospheric model used as the framework for the Eulerian mercury model is the Acid Deposition and Oxidant Model (ADOM) (39). Brief descriptions of the components of ADOM are found in Venkatram *et al*. (1988), Misra *et al*. (1989), Fung *et al*. (1991) and Fung *et al*. (1992). The adaptations of ADOM required to model atmospheric mercury are primarily in aqueous scavenging/chemistry and dry deposition (Petersen *et al*. 2001). The model includes elemental mercury, particulate phase mercury and divalent mercury species. Gas phase chemistry has not been included in this study since it is felt to be less important than aqueous chemistry. The transport and mixing

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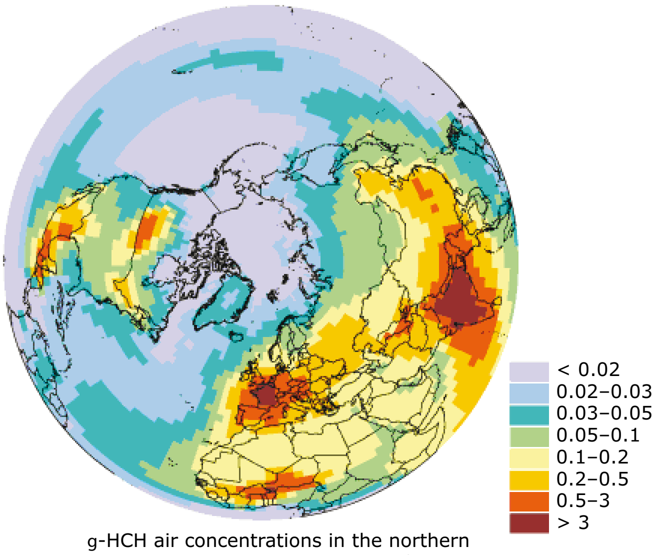
(36) The LCIA toxicity model IMPACT 2002. http://gecos.epfl.ch/lcsystems/Fichiers_communs/Recherche/IMPACT2002.html.

(37) Pennington DW, Margni M, Ammann C, Jolliet O (2005) Multimedia Fate and Human Intake Modeling: Spatial versus Nonspatial Insights for Chemical Emissions in Western Europe. Environmental Science and Technology 39:1119-1128.

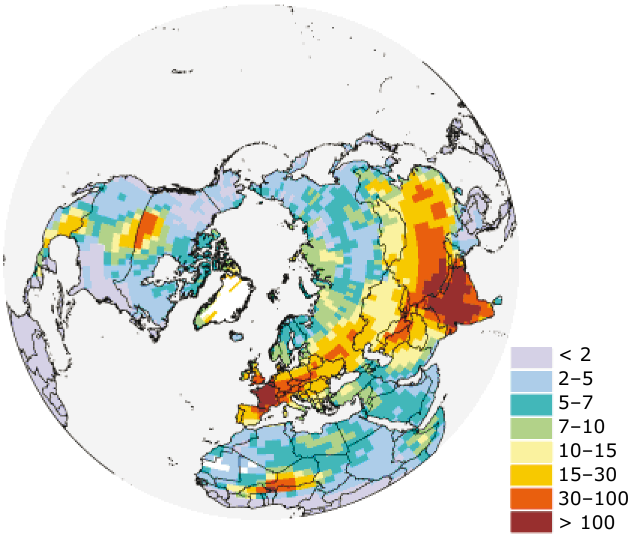
(38) European Environment Agency ERICA (European Rivers and Catchments) http://dataservice.eea.eu.int/dataservice/metadetails.asp?id=235.

(39) Bloxham, R. Modelling mercury atmospheric transport, chemistry and deposition. Proceeding of Canadian Mercury Network (1995). http://www.eman-rese.ca/eman/reports/publications/mercury95/part16.html.

Figure 7 Examples of EMEP hemispheric POPs model output — gamma HCH concentrations in air and vegetation



g-HCH air concentrations in the northern hemisphere for 1996, ng/m^3



g-HCH vegetation concentrations in the northern hemisphere in 1996, ng/g

aspects of ADOM were retained in the mercury model. As a first step in extending this model system for POPs the cloud mixing, scavenging, chemistry and wet deposition modules of ADOM have been restructured to accommodate recent developments in atmospheric processes of benzo(a)pyrene (B(a)P). A stand-alone version of these modules referred to as the Tropospheric Chemistry Module (TCM) was designed to simulate the meteorology and chemistry of the entire depth of the troposphere to study cloud mixing, scavenging and physico-chemical processes associated with precipitation systems that generate wet deposition fluxes of B(a)P). After comprehensive testing under different environmental conditions the TCM has been implemented into the full ADOM-POP model. Within the constraints of the available computer resources and input data, this model incorporates an up-to-date understanding of the detailed physical and chemical processes in the atmosphere. The vertical grid consists of 12 unequally spaced levels between the surface and the top of the model domain at 10 km. The model is run for a grid cell size 55 by 55 km (High resolution limited area model (HIRLAM) grid) over a 76 by 76 domain.

DEHM-POP

DEHM-POP model is based on the Danish Eulerian Hemispheric Model (DEHM), a three-dimensional dynamical atmospheric transport model. DEHM was originally developed to study the atmospheric transport of sulphur and lead into the Arctic, CO_2 and a chemical scheme with 60 components (40). In the horizontal plane, the model is defined on a regular grid using a polar-stereo graphic projection with a resolution of 150 km x 150 km at 60 ° N. The DEHM-POP domain was enlarged from 96 x 6 grid cells in the horizontal in the earlier versions of DEHM to 135 x 135 grid cells and it now extends into the Southern Hemisphere. The model has been used to estimate the distribution of alpha HCH in the Northern Hemisphere.

HYSPLIT 4

The HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory) model is the newest version of a complete system for computing simple air parcel trajectories to complex dispersion and deposition simulations (41) (42). As a result of a joint effort between NOAA and Australia's Bureau of Meteorology, the model has recently been upgraded. New features include improved advection algorithms, updated stability and dispersion equations, a new graphical user interface, and the option to include modules for chemical transformations. Without the additional dispersion modules, Hysplit computes the advection of a single pollutant particle, or simply its trajectory. The dispersion of a pollutant is calculated by assuming either puff or particle dispersion. In the puff model, puffs expand until they exceed the size of the meteorological grid cell (either horizontally or vertically) and then split into several new puffs, each with its share of the pollutant mass. In the particle model, a fixed number of initial particles are advected about the model domain by the mean wind field and a turbulent component. The model's default configuration assumes a puff distribution in the horizontal and particle dispersion in the vertical direction. In this way, the greater accuracy of the vertical dispersion parameterisation of the particle model is combined with the advantage of having an ever expanding number of particles represent the pollutant distribution. Hysplit will accept gridded input meteorological in a wide variety of formats that first have to be converted to standard ARL format. The model can be run interactively on the Web or the code executable and meteorological data can be downloaded to a Windows PC. A Mac version is available. Hysplit 4 has been evaluated for regional POPs modelling.

CMAQ Models-3

The Models-3 Community Multiscale Air Quality (CMAQ) modelling system has been developed under the leadership of the Atmospheric Modelling Division of the US EPA National Exposure Research Laboratory, NC. This new generation of modelling software, which is based on a Eulerian approach, was made available in June 1998 without charge for use by air quality regulators, policy makers, industry, and scientists to address multi-scale, multi-pollutant air quality concerns (43). Models-3, a flexible software framework, and its Community Multi-scale Air Quality (CMAQ) modelling system form a powerful third generation air quality modelling and assessment tool designed to support air quality modelling applications ranging from regulatory issues to science inquiries on atmospheric science processes. The CMAQ system can address tropospheric ozone, acid deposition, visibility, fine particulate and other air pollutant issues in the context of 'one' atmosphere perspective where complex interactions between atmospheric pollutants and regional and urban scales are confronted. CMAQ has been evaluated for regional POPs modelling.

3.3.5 *Inter-comparison of spatially resolved multimedia and large scale atmospheric models*

As can be concluded from the above discussion, there are a large number of multimedia and large scale atmospheric models now available. Existing models are being developed and improved and new approaches are under development in this active field of research. Because of the scarcity of monitoring data available with appropriate spatial and temporal resolution for all but a relatively small number of highly regulated chemicals, the issue of validating models by comparing predicted and measured environmental concentrations of chemicals is extremely problematic. A complementary strategy is to undertake inter-comparisons between model outputs for the same chemical and to evaluate uncertainty and the key factors that account for observed differences in outputs.

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(40) Hansen, K.M. *et al.* (2004). *Modelling atmospheric transport of persistent organic pollutants in the northern hemisphere with a 3-D dynamical model: DEHM-POP*. Atmos. Chem. Phys. Discuss., 4, 1339–1370.

(41) Draxler, R.R. and Rolph, G.D., 2003. HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory) Model access via NOAA ARL READY Website (http://www.arl.noaa.gov/ready/hysplit4.html). NOAA Air Resources Laboratory, Silver Spring, MD.

(42) Rolph, G.D., 2003. Real-time Environmental Applications and Display sYstem (READY) Website (http://www.arl.noaa.gov/ready/hysplit4.html). NOAA Air Resources Laboratory, Silver Spring, MD.

(43) Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. EPA/600/R-99/030, March 1999. http://www.epa.gov/asmdnerl/CMAQ/CMAQscienceDoc.html.

A number of such inter-comparison exercises are now under way ([17], p.39) or have recently been reported. An expert group, established under the auspices of the OECD, has recently reported the findings from a generic inter-comparison study of nine multimedia models ([44]). The objective was to assess their applicability and reliability in determining long-range transport potential and overall persistence. The working group used two approaches: the first approach compared model results for a comprehensive set of hypothetical chemicals; the second approach (the results of which are expected to be published in 2006) evaluated the ability of models to identify chemicals that have high long-range transport potential and overall persistence.

By applying data analysis techniques that compare models over the full space of plausible chemical partitioning and degradability properties, the authors were able to show that among the nine different models, the ranking of chemicals according to overall persistence and, to a lesser extent, potential for long-range transport depended mainly on chemical properties. Significant differences between the models were shown to be restricted to certain regions of the chemical space. These differences could be identified by detailed analyses of the chemical space plots. Four regions of the chemical space plots in particular illustrated different results in the various models: (I) For chemicals with low volatility, high water solubility, and high half-life in water, it is important whether and how transport in water is taken into account by the model. (II) For chemicals that strongly bind to aerosols due to high octanol-air partition coefficient, it is important whether the aerosol-bound fraction is assumed to be degradable. (III) For chemicals with high octanol-water and low air-water partition coefficients, particle-bound settling to the deep sea reduces their long-range transport potential in global models containing oceanic water compartments. (IV) For very volatile chemicals, the distinction between target- and transport-oriented metrics is important. The authors suggest that no single best model exists for screening-level identification of chemicals with high persistence and long-range transport potential and that, with some reservations, most models agree well and can therefore be used interchangeably. They concluded, however, that model selection is not arbitrary but requires careful consideration of the question and the context of the assessment. All nine models, when used in the correct context, provided credible and useful descriptions of the complex interactions between the environment and chemical pollutants.

Further inter-comparison studies are under way under UNECE auspices on POPs and mercury modelling.

The first two stages of a POPs model inter-comparison coordinated by MSC-E have recently been published. The study compared 13 models predicting environmental concentrations of three PCB congeners (PCB-153, -28 and -180), including the MSC-E/EMEP model, DEHM, Hysplit-4 and CMAQ. The first stage of the work ([45]) describes: the modelling approaches used (including gas/particle partitioning in the atmosphere, dry and wet deposition, gaseous exchange between atmosphere and surfaces and degradation rates; values of physico-chemical parameters and the results of calculation experiments. The study showed that the models had adopted markedly different approaches and values for some parameters, but concluded that all were able to simulate the main processes determining the fate of POPs in the environment. The second stage of the study has recently been published ([46]). The author's concluded that the MSC-E/EMEP-POP model parameterisation and the description of POP transport and exchange processes were in line with other participating models. The comparison of results with available measurements for selected POPs revealed that the model's predictions of spatial and temporal variations were in reasonable agreement with observed atmospheric levels of pollution within the European region, but further development is required with respect to the description of atmospheric degradation and exchange processes with underlying surface, including the refinement of partition coefficients. The authors conclude that there is a need to refine official POP emission data, including emission totals, spatial distributions and seasonal variations.

([44]) Fenner, K., *et al.* (2005). Comparing Estimates of Persistence and Long-range Transport Potential among Multimedia Models. Environmental Science & Technology. 39, (7), 1932–1942.

([45]) MSC-E Technical Report 1/2004 'POP Model Intercomparison Study. Stage I. Comparison of Descriptions of Main Processes Determining POP Behaviour in Various Environmental Compartments' V. Shatalov; E. Mantseva; A. Baart; P. Bartlett; K. Breivik; J. Christensen; S. Dutchak; D. Kallweit; R. Farret; M.F edyunin; S. Gong; K.M. Hansen; I. Holoubek; P. Huang; K .Jones; M. Matthies; G. Petesen; K. Prevedouros; J. Pudykiewicz; M. Roemer; M. Salzman; M. Sheringer; J. Stocker; B. Strukov; N. Suzuki; A. Sweetman; D. van de Meent; F. Wegmann.

([46]) EMEP/MSC-E Intermediate Technical Report 7/2005 August 2005 'POP Model Intercomparison Study. Stage II. Comparison of Mass Balance Estimates and Sensitivity Studies' Shatalov, V., Gusev, A.; Dutchak, S.; Holoubek, I.; Mantseva, E.; Rozovskaya; O.; Sweetman, A.; Strukov, B.; Vulykh N.

Parallel measurements of POPs in air and other environmental compartments and information on measurement data uncertainties are also required.

The main task of the mercury modelling inter-comparison (47) was to assess the capability of seven models to reproduce measurements of mercury concentrations in air and precipitation and to get a clear idea of range of uncertainties of results obtained by modern models. The models compared included MSC-E/EMEP heavy metal model (regional and hemispheric), Hysplit, ADOM, CMAQ and DEHM. The third stage of the project was aimed at comparisons of modelling results with long-term (month — year) observations. The most important constituent of the third stage was an attempt to compare capabilities of the participating models to simulate integrated items of mercury atmospheric balances for individual countries. Just such calculations are of the particular interest from an ecological viewpoint and for the implementation of Heavy Metal Protocol to the Convention on Long-range Transboundary Air Pollution. There are no more than about a dozen mercury models designed for evaluation of mercury atmospheric transport on regional (continental) and global levels. Most of them partly or fully participated in the project. They are different in many aspects: in methods of atmospheric transport simulation (Eulerian or Lagrangian types), in approaches to simulate deposition mechanisms, and in the representation of mercury chemistry in the atmosphere. The main interest of the study is focused on European region (EMEP domain) but some models consider mercury fate on a hemispheric level. Accordingly, spatial resolution of the models is different, both horizontally and vertically. Model outputs were compared with results of routine monitoring of mercury in the atmosphere and in precipitation. Different models used input meteorological information obtained and prepared individually. Some of the models additionally simulate chemical reactants involved in mercury chemistry (ozone, sulphur dioxide), while some of the models use predetermined concentration values of such reactants.

The study found a number of areas where significant differences between models were seen. It also revealed some important gaps in knowledge, particularly in relation to natural sources of mercury and its speciation in the atmosphere. The physico-chemical properties of gaseous compounds of oxidised mercury are poorly known and correspondingly, parameterisation of scavenging processes for such compounds needs significant improvement.

We concluded therefore that at the present state of knowledge, it is not possible to provide a general recommendation for the use of any one of these widely-used multimedia or large scale atmospheric model for POPs or mercury over another.

Application of spatially-resolved multimedia and large scale atmospheric models to EPER emission sources

There are several spatially-resolved multimedia and large-scale atmospheric models that could potentially be used to map environmental concentrations of chemicals released from EPER sources. Of these, the suite of models which has gained the highest level of establishment in terms of monitoring compliance with international agreements on the transboundary transport of air pollutants are the regional and hemispheric EMEP models used for predicting the distribution and deposition of certain POPs and heavy metals. The models have also been subject of extensive international peer review and have been assessed in several inter-comparison studies with models capable of similar purposes. The emission input data for the EMEP models are regional emission data, based on national inventory data or, where this is lacking, expert judgement. We are not aware that EMEP models have been used for individual point source emissions, although there would appear to be no scientific reason why they could not be so used. The regional models would be more relevant in this application than the hemispheric version, as the smaller grid size in the former would be more appropriate for point source assessment, as opposed to regional emissions. However, for individual point sources of pollutants, where the highest concentrations are localised to within a few km of the source, the grid size used in EMEP would be too coarse to resolve local concentration gradients.

The EMEP models are not currently available for use outside MSC-E, although some form of the models may become available in the future. The models run on a standard specification PC. It may be possible, however, to negotiate the use of EMEP models for regional modelling of specific EPER substances

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(47) MSC-E Technical Report 1/2005 'Intercomparison Study of Numerical Models for Long-range Atmospheric Transport of Mercury. Stage III. Comparison of modeling results with long-term observations and comparison of calculated items of regional balances' A. Ryaboshapko; R. Artz; R. Bullock; J. Christensen; M. Cohen; R. Draxler; I. Ilyin; J. Munthe; J. Pacyna; G. Petersen; D. Syrakov; O.Travnikov.

from point sources under contract with MSC-E. Any such application would need to be consistent with MSC-E's terms of reference and avoid conflicting with their duties under EMEP and the CLTAP.

A number of the models reviewed here have been (or are being) assessed with the EMEP models as part of a model inter-comparison exercise. The conclusions from such inter-comparison are generally that all the models assessed are capable of fulfilling the purposes for which they were applied: no clear 'best' model has been identified. In the absence of a clearly preferred model there would appear to be no over-riding scientific reason to prefer one model to another.

Amongst the models assessed, there are several new atmospheric models available to users via the Internet or web download that appear to be extremely promising and which have been assessed against EMEP under the inter-comparison studies. These models are Hysplit 4 and the CMAQ-Models-3 programmes, developed in the United States. Both models have been subject to extensive peer review and are well established in the United States as highly flexible modelling tools with a wide range of applications. Their accessibility is a considerable advantage over EMEP, but of course they do not have the multimedia capability of EMEP and other true multimedia models.

However, in the absence of a model clearly preferred on scientific grounds, a reasonable choice for the modelling of POPs and metals from EPER sources would be the regional EMEP models. As these models are the established tools for reporting regional distribution of chemicals under the CLTAP, it would be important to show consistency in mapping the effects of point sources by the same methodology. If a different model were used, it would be highly problematic if there were a model-generated divergence in the distribution of chemicals from modelled point sources, compared with EMEP predictions for regional emissions, notwithstanding concerns over the accuracy of the EMEP model predictions raised above. However, as we will propose in Chapter 4 there is a more cost-effective solution for predicting the chemical density of Europe than modelling with complex, data-hungry models. But before developing these arguments, we will first complete this review of models by considering those applied to surface waters and sewage treatment works.

3.4 Surface water models

Table 16 lists as selection of several models for predicting partitioning of chemicals released to surface water from point source discharges. The multimedia screening models (including EUSES) discussed above also have application in this area. The list excludes a large number of other models that have been developed for application to diffuse sources (such agricultural run-off of nutrients and pesticides) as the focus of the present feasibility study is on industrial point sources such as those listed in EPER. Examples of recent work on models for diffuse sources include the various models evaluated under the Euroharp programme and the Steps 1–2 model developed by the European Commission's Joint Research Centre for pesticide risk assessment.

The level of documentation and application history for the models in Table 16 has been assessed using the three-level scale shown in Table 4. The models are described in further detail below. The models require a standard level PC running under Microsoft Windows®.

There are also numerous aquatic models designed for hydrological modelling, sediment transport, storm water run-off prediction, chemical or oil

Table 16 Surface water models

Model	Chemicals	Availability	Levels of documentation	Application history
GREAT-ER	Organic or inorganic	Free download http://www.great-er.org/pages/Downloads.cfm	1	1
GEMCO	Organic or inorganic (except metals, other adsorbing species and volatile compounds)	Free CD from http://www.wldelft.nl	1	3
AQUATOX	Organic or inorganic	Free download http://www.chemmap.com/	2	2
CHEMMAP	Organic or inorganic	Commercial http://www.chemmap.com/	2	2

Table 17 Other surface water models

Model	Description	Availability
SMPTOX	Sponsored by US EPA, this model calculates water column and stream bed toxic substance concentrations resulting from point source discharges into streams and rivers. It predicts pollutant concentrations in dissolved and particulate phases for water column and bed sediments and total suspended solid. Separate simulation routines are provided for model calibration, waste load allocation, and sensitivity analysis. Version 2.01 is current, released October 1993. MS-DOS	Free download from US EPA: http://www.epa.gov/ceampubl/swater/smptox3/index.htm
QUAL2K	QUAL2K (or Q2K) is a 1 dimensional river and stream water quality model for well-mixed channels with steady state hydraulics. Non-uniform, steady flow is simulated. The model is used for simulating conventional pollutants (Nitrogen, Phosphorus, Dissolved Oxygen, BOD, Sediment Oxygen Demand, Algae), pH, Periphyton, Pathogens. Applications for other chemicals are not reported. Current version (v3.22) released May 1996.	Free download from US EPA http://www.epa.gov/athens/wwqtsc/html/qual2k.html
CORMIX	Cornell Mixing Zone Expert System (CORMIX) is a US EPA-supported water quality modelling and decision support system designed for environmental impact assessment for simulating a site-specific discharge configuration. A mixing zone is a limited area where initial dilution of a discharge takes place and where numeric water quality criteria can be exceeded but acutely toxic conditions are prevented. Use appears limited to conventional water quality pollutants. Cormix v4.3 released October 2004. MS-DOS	Download available for purchase from Cormix homepage: http://www.cormix.info/
PLUMES	Plume dispersion model for modelling aquatic discharge dispersion to marine and some freshwater bodies Both buoyant and dense plumes, single sources, and many diffuser outfall configurations can be modelled. The current version (v3.0) was released in 1994.	Free download from US EPA http://www.epa.gov/ceampubl/swater/plumes/index.htm
GCSOLAR	GCSOLAR computes direct photolysis rates and half-lives of pollutants in the aquatic environment., calculated as a function of season, latitude, time-of-day, depth in water bodies, and ozone layer thickness. Current version (v1.2) released June 1999. MS-DOS.	Free download from US EPA http://www.epa.gov/ceampubl/swater/gcsolar/index.htm
BASINS	BASINS is a multipurpose environmental analysis system designed for use by regional, state, and local agencies in performing watershed and water quality-based studies. Installed on a personal computer, BASINS allows the user to assess water quality at selected stream sites or throughout an entire watershed. The BASINS GIS database is specific to the United States.	Free download from US EPA http://www.epa.gov/waterscience/basins/basinsv3.htm
SCREMOTOX	North Sea specific, taking into account transport and retention within river systems, estuaries and North Sea mixing zones, using a grid comprising 3 915 computational elements (DELWAQ). In addition to PECs based on estimated emissions from EC production and use figures, the methodology allows indirect emissions from the atmosphere and direct marine emissions to be modelled and monitoring data to be included. Provides ranking of substances based on PEC/PNEC.	http://www.wldelft.nl/proj/pdf/3uk00101.scherm.pdf
EXAMS	EXAMSII is an interactive modelling system that allows a user to specify and store the properties of chemicals and ecosystems, modify either via simple commands, and conduct rapid evaluations and error analyses of the probable aquatic fate of synthetic organic chemicals. EXAMS combines chemical loadings, transport, and transformation into a set of differential equations using the law of conservation of mass as an accounting principle. It accounts for all the chemical mass entering and leaving a system as the algebraic sum of external loadings, transport processes that export the compound from the system, and transformation processes within the system that convert the chemical to daughter products. The programme produces output tables and simple graphics describing chemical exposure, fate, and persistence. Current version v2.98.04.06 was released in April 2005.	Free download from US EPA http://www.epa.gov/ceampubl/swater/exams/ US EPA (1997a) (48)

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(48) US EPA. 1997a. EXAMS. Exposure Analysis Modeling System. US-EPA, Centre for Exposure Assessment Modelling, Athens, GA, USA.

Model	Description	Availability
MAM PEC Model	The 'Marine Antifoulant Model' predicts environmental concentrations of antifouling products in five generalized 'typical' marine environments (open sea, shipping lane, estuary, commercial harbour, yachting marina). The model takes into account emission factors (e.g. leaching rates, shipping intensities, residence times, ship hull underwater surface areas), compound-related properties and processes (e.g. Kd, Kow, Koc, volatilization, speciation, hydrolysis, photolysis, bacterial degradation), and properties and processes related to the specific environment (e.g. currents, tides, salinity, DOC, suspended matter load). Default QSAR approaches to estimate missing data are included. It is specific to paint emissions.	Available from http://www.wldelft.nl/rnd/intro/topic/mampec/
PROTEUS	'Pollution Risk Off-shore Technical EvalUation Systems' assesses dispersion and behaviour of drilling and production discharges from off-shore oil and gas platforms. The model supports the following risk assessment methods: PEC/PNEC, critical body residues, whole effluent toxicity scheme. It is specific to platform discharges.	BMT Marine Information Systems (1999). Available commercially from http://www.bmtcordah.com/services/consultancy.aspx?id=44
DREAM	'Dose related Risk and Effect Assessment Model' This model assesses the environmental risks from water discharges into the ocean. Plumes of discharged chemicals are modelled in a three-dimensional time dependent concentration field (PEC). Risk can be determined in several ways: 1) as RCR comparing the modelled PEC with PNEC (TGD method), 2) as time variable RCR based on the modelled PEC and exposure dependent PNEC and 3) based on body burden and critical body burden ratios. Present version of DREAM does not include the latter, which is still to be developed. DREAM offers the possibility of risk assessment of mixtures, total risk is the sum of the risk of each sub-group of compounds. Risk is presented as three-dimensional, time variable risk maps.	Johnsen *et al*., 2000 ([49]) http://www.sintef.no/static/ch/environment/dream/dream.htm
ECOFATE	EcoFate is for conducting ecosystem-based environmental and ecological risk assessments of chemical emissions by point and non-point sources in freshwater and marine aquatic ecosystems, including lakes, rivers and marine inlets. It is designed to assess the cumulative impact of chemical inputs in terms of contaminant concentrations in water, sediment and biota of an entire ecosystem and to interpret these concentrations in terms of exceedance of environmental criteria and standards, potential for toxic effects in biota of the ecosystem and risks to human beings exposed to contaminated fish products or contaminated water.	http://www.rem.sfu.ca/ecofate/ecofate.html

spill modelling and anti-fouling agent dispersion shown in Table 17, which are not generally relevant to chemical fate modelling. These models have been excluded from further analysis here. Table 17 also lists a number of older chemical models and specialist modelling tools available for specific related purposes, such as mixing of discharge plumes and for calculating aquatic photolysis rates of chemicals. Many of these older models run on Microsoft DOS rather than Windows.

The surface water models considered to have the greatest potential application for chemical fate modelling are described below.

GREAT-ER

GREAT-ER is a geographically referenced exposure assessment tool for European rivers ([50]). It is a GIS-based model for environmental risk assessment and management of chemicals in river basins. GREAT-ER provides a higher tier support system designed for use at a post-screening level in the EU Risk Assessment process, and in the EU Water Framework Directive. It combines a GIS (Geographic Information System) with fate models to produce a simple and clear visualisation of predicted chemical concentrations and water quality along a river. GREAT-ER is a tool to study the impact of chemicals emitted by point sources

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([49]) Johnsen, S., Frost, T.K.; Hjelsvold, M.; Utvik, T.I., 2000. The Environmental Impact Factor — a proposed tool for produced water impact reduction, management and regulation. SPE paper 61179, presented at the 2000 HSE meeting, Stavanger, Norway.

([50]) GREAT-ER — Contribution of the European Chemicals Bureau, Institute for Health and Consumer Protection (IHCP), Joint Research Centre to the development of a Geo-referenced Regional Exposure Assessment Tool for European Rivers. Final Report Christian J.A. Heidorn, October 1999 Contract No.: 11677-96-02 T1ED ISP B http://www.great-er.org/files/ECB_greater_finalreport.pdf See http://www.great-er.org/files/GREAT-ER-Related_Publications.pdf for list of publications up to May 2002. http://www.great-er.org/pages/GenericSubPage.cfm?pageId=31&parentPgId=2 Download http://www.great-er.org/pages/Downloads.cfm Equations http://www.great-er.org/files/great-er_model_equations.pdf.

into rivers for calculating GIS-based equivalents of 'PEClocal' and 'PECregional' for the aquatic environment in a probabilistic way. It has already been implemented for a variety of river basins: four in the United Kingdom (Aire, Calder, Went, and Rother), one in Italy (Lambro), four in Germany (Itter, Unter-Main, Main and Rur), one in Belgium (Rupel) and one in France (Mayenne). Several other river basin applications are under development. GREAT-ER has been developed by a multi-agency European consortium from industry, regulators and academia. The GREAT-ER desktop comes with 16 GIS datasets of European catchments as standard. Other catchment datasets are in preparation. The user may also provide data specific for other catchments. GREAT-ER has been validated in several catchments for a range of organic and inorganic chemicals. The model is available for free download for use on Windows-based PCs. A programme of work is under way to include an additional model (TERRACE) dealing with diffuse sources, including deposition from the atmosphere to the aquatic environment, within the GREAT-ER framework (51). Regulatory bodies in Germany and United Kingdom have provided data and financial support for GREAT-ER catchment development and validation projects on a large spatial scale.

GEMCO

GEMCO (Generic Estuary Modelling of COntaminants) is a generic steady-state screening level model for European estuaries, developed by a consortium led by Delft Hydraulics funded by CEFIC's Long-range Research Initiative. The model, which was released in 2004, calculates chemical concentrations in water, sediment and biota in a generic user-defined estuary. There are three levels of detail. The first level provides four different generic 'annual averaged' estuaries. In the second level the user can select the seasonal scenarios for the generic estuaries and the third level provides access to over 100 specific estuaries. The model calculates the output of the chemical(s) of interest to the marine environment at the end of estuary and a supplementary module uses this value as an input parameter for the marine plume calculation (based on the requirements of the technical guidance document) following the recommendations for adjustment to EUSES in the TGD. GEMCO is suitable for persistent organic chemicals and general organic chemicals although half-life needs to be known as an input variable or the model will provide an output based on no degradation. The model is not suitable for highly volatile chemicals or for metals. It does not take ionic adsorption to clays into account. GEMCO is freely available on CD-ROM from Delft Hydraulics (52). The model has been peer reviewed but has not yet been officially approved for risk assessment in the marine environment. Validation tests so far indicate that the model can predict actual concentrations to within +/– 20 % of measured values.

AQUATOX

AQUATOX (53) is a PC-based ecosystem model developed for the US EPA that simulates the transfer of biomass and chemicals from one compartment of the ecosystem to another. It was developed for ecological risk assessment of pesticides. It does this by simultaneously computing important chemical and biological processes over time. AQUATOX can predict not only the fate of chemicals in aquatic ecosystems, but also their direct and indirect effects on the resident organisms. Therefore it has the potential to help establish the cause and effect relationships between chemical water quality, the physical environment, and aquatic life. AQUATOX can model inputs from point sources, diffuse sources and from the atmosphere. It can be combined with hydrodynamic/GIS models. It has been used to model bioaccumulation of PCBs in the Housatonic River for the US government, in a PCB bioaccumulation project in The Netherlands and various other maximum daily load and pesticide fate studies. AQUATOX simulates the behaviour of numerous inter-related components in lakes, reservoirs, ponds, rivers, and streams: including algae and submerged aquatic vegetation; benthic invertebrates, zooplankton, and fish; nutrients and dissolved oxygen; sediments and toxic chemicals. The model itself, the modelling framework design and quality assurance project plan may be downloaded free of charge. The model runs on Windows-based PCs.

CHEMMAP

CHEMMAP (54) chemical discharge model system is a three-dimensional model designed to predict the trajectory, fate, impacts and biological effects of a wide variety of chemical substances released from point sources or spills. It includes initial plume dynamics, volatilisation, adsorption and desorption of chemicals to sediments, transport and dispersion of dissolved and suspended matter in the water column and atmosphere, decomposition.

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(51) For information on the TERRACE model, see: http://www.silsoe.cranfield.ac.uk/iwe/projects/terrace/terrace.htm.

(52) http://www.wldelft.nl.

(53) AQUATOX — A model for ecological risk assessment of pesticides and references therein. http://www.myweb.cableone.net/dickpark/AQTXFacts.htm. Download version 2 from EPA http://www.epa.gov/ost/models/aquatox/

(54) Commercially available from Applied Science Associates, inc. http://www.chemmap.com/.

It is commercially available from the developers, Applied Science Associates, inc.

3.4.1 *Input data requirements and outputs for surface water models*

Basic data is required on the physicochemical properties of the substance of interest (i.e. partition coefficients, vapour pressure, solubility, biodegradability etc.), the nature of the discharge (e.g. quantities, flow rate, temperature etc.) and the nature of the receiving water body (e.g. flow rate, sediment burden, physiography, water quality etc.). Outputs consist of predicted concentrations in water, sediment and air. In the case of GREAT-ER, these are spatially resolved and may be used directly as local and regional predicted environmental concentrations.

3.4.2 *Application of surface water models to EPER emission sources*

In principle, any of the above models that predict environmental concentrations from discharge data may be used with EPER release data for direct emissions to water. The EUSES screening model described in Section 3.3.3 also generates these outputs for chemicals released to water. For post-screening applications, the GREAT-ER model would be the first choice as it has been extensively evaluated and tested for this specific purpose within the EU regulatory framework. Also of interest would be the AQUATOX model, which in addition to chemical fate modelling can also predict the impacts on biota and aquatic community structure. This model does not have such an extensive record of validation in a European setting for chemical fate modelling as GREAT-ER. Application for biotic and community impacts would require data of European species representative of the region under study.

3.5 Sewage treatment models

EPER lists releases to water as 'direct' and 'indirect' releases. Direct releases are those in which the substance in question is released directly to the receiving water body (river, estuary, lake, sea etc.). Indirect releases are made from facilities via a sewer to an off-site industrial or municipal wastewater treatment plant. Further reduction in the pollutant load then takes place before the treated effluent is released into the receiving water body.

Models of sewage (i.e. wastewater) treatment works allow the fate of chemicals in the indirect releases to be calculated. Models calculate:

- how much of the incoming substance is biodegraded;
- how much is adsorbed to sludge (and so may be deposited to soil if the sludge is used for soil application);
- how much is volatilised; and
- how much is released in the treated effluent.

Models vary in terms of the size of their chemical database, the number and types of the unit processes and other features. Simpler models use pseudo-first order reaction kinetics to simulate biodegradation. Other models use mixed order kinetic ('Monod' kinetics) to simulate decomposition rates at high concentrations. Details of equations used for modelling air emissions from wastewater treatment are given in a review document published by the US EPA (55).

A selection of models for sewage treatment plants is given in Table 18, evaluated according to the three-level system shown in Table 4. The models are described below. The list excludes numerous models that focus on the hydrodynamics of sewage treatment plants and those that just deal with classic water quality indicators such as total N, P, BOD, COD or dissolved oxygen, or odour emissions from treatment works.

SIMPLETREAT
SIMPLETREAT (56) was developed as a box model to assess the fate of chemicals for' base-set' data as requested by the European Commission for the notification of new chemicals, available as an Excel® spreadsheet. SIMPLETREAT can be used as a diagnostic tool, providing regulatory authorities with a quick impression of the emission patterns of a chemical in a municipal wastewater treatment plant. It requires a minimal data input to calculate air-water and sludge solids-water partition coefficients. Distribution coefficients are calculated

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(55) Air emission models for waste and wastewater. US Environmental Protection Agency contract No 68D10118, November 1994, report No EPA 453-R-94-080A. http://www.epa.gov/ttn/chief/software/water/air %20emission %20models %20for %20waste %20and %20wastewater.pdf.

(56) Struijs, J., Stoltenkamp, J., and van de Meent, D. (1991). A spreadsheet-based box model to predict the fate of xenobiotics in a municipal wastewater treatment plant. Water Research 25, 891–900.

Table 18 Sewage treatment plant models

Model	Chemicals	Availability	Levels of documentation	Application history
SIMPLETREAT	Organics	Contact developer	1	1
WWTREAT	Organics	Contact developer	2	2
WATER9	Organics	Free download www.epa.gov/ttn/chief/software/water/	1	2
TOXCHEM+	Organics and metals	Commercial www.enviromega.com/toxplus3.htm	1	2
STP	Organics	Free download www.trentu.ca/cemc/models/STP210.html	2	2

from solubility, vapour pressure, and octanol-water partition coefficients, or actual measured partition coefficients can be entered. Biodegradability data and the degree of dissociation or protonation are the required input data to account for degradation and speciation changes of the chemical in the water phase. An improved version of SIMPLETREAT is incorporated into the EUSES multimedia screening model described in Section 3.3.3. It is used for calculating steady-state concentrations in a sewage treatment plant, consisting of a primary settler, an aeration tank and a liquid-solid separator. With SIMPLETREAT, the sewage treatment plant is modelled for an average size treatment plant based on aerobic degradation by active sludge, consisting of nine compartments. Depending on the test results for ready and/or inherent biodegradability of a substance, specific first order biodegradation rate constants are assigned to the compound. An improved process formulation for volatilisation from the aeration tank, which is also applicable to semi-volatile substances, has been incorporated in the revised version.

WWTREAT

WWTREAT model (57) was developed to predict the degree of removal and distribution of consumer product chemicals among air, treated liquid effluent, and sludge for primary and activated sludge wastewater treatment plants using independently determined distribution coefficients and biodegradation rate constants. The major difference between this model and previous models based on removal of BOD is that it assumes that the total chemical, and not just the dissolved fraction, is available for biodegradation.

WATER9

WATER9 is a Windows-based model available for download free of charge from the US EPA Clearinghouse for Emission Factors and Inventories. The current version (version 2.0) was released on 1 July 2004. It supersedes WATER8, Chem9, and Chemdat8, and WATER9 version 1.0. It consists of analytical expressions for estimating air emissions of individual waste constituents in wastewater collection, storage, treatment, and disposal facilities; a database listing many of the organic compounds; and procedures for obtaining reports of constituent fates, including air emissions and treatment effectiveness. WATER9 contains a set of model units that can be used together in a project to provide a model for an entire facility. WATER9 is able to evaluate a full facility that contains multiple wastewater inlet streams, multiple collection systems, and complex treatment configurations. WATER9 provides separate emission estimates for each individual compound that is identified as a constituent of the wastes. The emission estimates are based upon the properties of the compound and its concentration in the wastes. To obtain these emission estimates, the user must identify the compounds of interest and provide their concentrations in the wastes. The identification of compounds can be made by selecting them from the database that accompanies the program or by entering new information describing the properties of a compound not contained in the database. Many studies have been conducted on previous versions of WATER9 (i.e. WATER7 and WATER8), comparing predicted VOC emissions from various water treatment facilities with measured data (see the review published by Environment Canada (58), and

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(57) Cowan, C.E.; Larson, R.J.; Feijtel, T.C.J. and Rapaport, R.A. (1993). An improved model for predicting the fate of consumer product chemicals in wastewater treatment plants.Water Research, **27** (4), 561–573.

(58) Environment Canada National Pollutant Release Inventory Guidance Manual of the Wastewater Sector. http://www.ec.gc.ca/pdb/npri/2002guidance/WW2002/WW_2002_annexI_e.cfm.

references therein). WATER9 has the ability to use site-specific compound property information, and the ability to estimate missing compound property values. Estimates of the total air emissions from the wastes are obtained by summing the estimates for the individual compounds. The EPA document, 'Air Emissions Models for Waste and Wastewater'55 includes the equations used in the WATER9 model.

TOXCHEM+
TOXCHEM+ (version 3, treatment and collection). TOXCHEM+ is an US EPA-approved, emission-estimating program. It is used to determine emissions of contaminants (organic and metallic) from wastewater treatment and collection systems. It is particularly suited for synthetic/organic chemical, pharmaceutical, and pulp and paper industries. TOXCHEM+ was developed by the Wastewater Technology Centre of Environment Canada and Enviromega and is commercially available from Enviromega's website. The principle used by TOXCHEM+ for emission estimation is based on modelling the fate of pollutants in treatment and collection systems. This includes sorption to solids, volatilisation to air, and biodegradation in liquid. TOXCHEM (the previous version of TOXCHEM+) includes both steady-state and dynamic models to predict locations and quantities of VOC emissions within a wastewater treatment facility. It contains a database of more than 200 substances and allows for user-specified substances. Many evaluative studies have been conducted on the use of TOXCHEM+ and the previous version, TOXCHEM as described in the summary review published by Environment Canada.

STP model
The STP model (sewage treatment plant) version 2.10 has been developed by the Canadian Environmental Monitoring Centre (CEMC) of Trent University. Details of the model are available from the developer's website ([59]) and are summarised here. The model is available free of charge from CEMC in both Windows and DOS versions. The current version (2.10) was released on 10 August 2004. It supersedes the previous release (v. 1.5, released October 2001) and has improved functionality, user-friendliness, flexibility and improved display of output. The STP model estimates the fate of a chemical present in the influent to a conventional activated sludge plant as it becomes subject to evaporation, biodegradation, sorption to sludge and to loss in the final effluent. The most critical and uncertain variable is the biodegradation rate constant and its dependence on biomass concentration.

The model is useful for establishing the general features of a new or existing chemical's behaviour, in a sewage treatment plant. It is not intended as an accurate simulation of chemical fate in a specific plant, rather it is a screening level model which seeks to estimate the likely proportions of the chemical which leave the system by biodegradation, in sludge, by evaporation, and in the water outflow. These proportions are dictated by both the physical chemical properties of the substance and the characteristics of the treatment plant. The effect of varying chemical properties such as half-lives and operating conditions can be readily explored. Details of the programme have been published in the peer-reviewed literature ([60]).

3.5.1 Input data requirements and outputs for sewage treatment models

Depending on model complexity, the input data requirements relate to the design and operational characteristics of the sewage treatment facility and the properties of the chemical of interest. At a minimum, these will include factors such as capacity of the STP, wastewater per inhabitant, population, surplus sludge per inhabitant and suspended solid loading in influent. The basic chemical properties are Henry's law constant, octanol-water partition coefficient and the first-order rate constant for biodegradation. The output data will include predicted concentrations in air, effluent and sludge. The effluent concentration may feed into a surface water model for determining subsequent fate of the chemical following its discharge for the treatment plant.

3.5.2 Application of sewage treatment models to EPER emission sources

Any of the above models may be used with EPER 'indirect releases to water' data. SIMPLETREAT, as represented in EUSES and STP model may be considered as screening models. More detailed analysis may be undertaken with TOXCHEM+ and WATER9, which appear to allow a more detailed characterisation of the treatment plant.

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[59] Canadian Environmental Modelling Centre http://www.trentu.ca/cemc/models/STP210.html.
[60] *Environ. Sci. Technol. Vol. 29, p. 1488, 1995 by Clark, B.; Henry, J.G. and Mackay, D.*

3.6 Conclusions from Phase 1

The following conclusions can be drawn from Phase 1 of this feasibility study:

1. Predicting the chemical density of Europe from emissions data will require access to appropriate models and the data needed to drive them.
2. A large number of models are available for predicting environmental concentrations of chemicals in single or multiple environmental media. Many of these models are well-established in terms of history of usage in policy or regulatory applications, have been peer-reviewed and used as the basis of many peer-reviewed scientific papers. Most of these models are readily available, either for purchase or as freeware. Most will run on current Microsoft Windows® based personal computers commonly in general use and some may be run interactively over the Internet. A few require a more sophisticated platform, such as Unix or Linux workstations. Some established models, notably EMEP models, are not publicly available, at least at present.
3. Models range from highly complex spatially and temporally resolved models capable of predicting small scale variations in chemical concentrations in one or more environmental media, to simpler screening tools that predict concentrations averaged over wider spatial and temporal domains. A number of leading models have been identified for specific applications that are particularly well-established and which could form the basis of a set of tools for modelling chemical density from emissions data. The study has not attempted to identify the 'best' model for any particular purpose: this is outside the current remit and would be a major task in its own right. A number of inter-comparison studies have been completed, or are under way under the auspices of EMEP for several well-established multimedia models for regional/hemispherical modelling of POPs and mercury. These have not so far established clear benefits of one model over another.
4. A wide range of factors determines the fate of chemicals in the environment. These factors relate to the process of the release itself and how the substance is dispersed into the receiving medium; the properties of the chemical that determine its persistence and mobility (such as vapour pressure, partition coefficients, degradation rate constants in various media, etc.); meteorological and hydrological factors spatially and temporally disaggregated at the appropriate level that affect the dispersion of the substance and also landscape characteristics (also spatially and temporally disaggregated) such as vegetation type, coverage, land use, etc. Local scale air dispersion models, for example, need detailed information on the release characteristics and local topography and meteorology at the time of release: spatially-resolved multimedia models require a full set of input data relating to the factors listed above.
5. On the other hand, screening type models have much lower requirements for input data and usually characterise the receiving environment in terms of broad average landscape properties, meteorology and hydrology. A screening model, EUSES, has been endorsed by the European Commission for chemical risk assessment in compliance with the requirements of its official technical guidance. It is important to note that highly detailed models will not provide greater accuracy of output than a simpler screening model unless the input data is characterised with the required degree of certainty.
6. It is anticipated that a great deal of effort would be required to predict the chemical density of Europe through detailed modelling of all EPER releases. In addition to the highly resource-intensive work needed to run detailed models and to assess and interpret the results correctly, a more important constraint is the difficulty in accessing key data on the specific releases and local dispersion. A strategy to use a combination of screening and detailed modelling has been developed as part of the second phase of this study, described in the next section.

4 Phase 2 — Strategy, demonstration and proposals for development

This second phase of this feasibility study addresses Tasks 6 to 8 of the technical specification (Appendix 1). It commences with a strategic proposal for using models to predict the chemical density of Europe, based on emission data contained in EPER. This work element corresponds with Task 8 in the technical specification. The strategic plan determines the direction and approach needed for the model test runs (Task 6) and development of a draft work plan (Task 7). It is therefore logical to describe the strategic plan before reporting on these other two tasks.

The strategy was discussed as part of the peer review of a draft of this final report at the expert workshop held on 16 August 2005 (see Appendix 4) for the workshop proceedings). Workshop delegates endorsed the overall approach outlined in the preferred option described below, subject to some specific recommendations for revision. The strategy presented here is based on the original peer-reviewed version as it raises a number of important issues relating to how information on chemical concentrations local to emission sources could be generated, given the difficulty in obtaining the site-specific details needed for accurate modelling at this geographical scale. The work plan for implementing the preferred option (described in Section 4.3) has, however, been revised to take account of the recommendations suggested at the workshop, as well information from the evaluation of the preferred option described in Section 4.2. Overall conclusions from this second phase of the feasibility study are given in the final part of this section.

4.1 Strategy development

From consideration of the findings from the model evaluation undertaken in the first part of this feasibility study, two main alternative strategies for mapping the chemical density of Europe (Task 8) have became apparent:

Option 1: detailed modelling approach. This would involve:

- establishing a programme of detailed modelling based on a list of priority EPER substances.
- choosing a selection of detailed models according to the substances of interest from the most established models identified above.
- gathering extensive datasets on emissions, chemical properties and speciation of emissions (including congener profiles of POPs), local and regional landscape parameters, meteorological information.
- running the models.
- evaluating the outputs and correcting for any apparent anomalies.
- re-configuring input data and model parameters.
- re-running the models.
- publishing the results (on the Internet).

Option 2: staged modelling approach. This option would require:

- using a well-established screening model to undertake a preliminary prediction of environmental concentrations from EPER emission data. (As the EU's established risk assessment tool, EUSES would be a good choice).
- preparing regional and local predicted environmental concentrations based on either default or better estimates of releases, physicochemical properties, congener mix, landscape etc. The calculated concentrations will generally be highly conservative.
- presenting the information.
- informing industry and member state competent authorities of the outcome of these assessments.
- allowing industry to submit revised estimates provided that the methodology is transparent and the information is given on an 'open book' basis and is hence open for public scrutiny. Models used by industry should meet criteria relating to model documentation, peer review studies and validation. The model assessment

carried out in the previous chapter of this report will be helpful in selecting models that are 'fit for purpose'.

- commissioning EMEP MSCE or contractors to carry out more detailed modelling or monitoring where regional concentrations (i.e. not attributable to single source) exceed benchmarks. Again, the model assessment carried out in the previous chapter of this report will be helpful in selecting models that are 'fit for purpose'.
- revise the predicted concentrations taking account of information provided by industry or the national regulators and the results of detailed modelling.
- publishing the predicted concentrations on the Internet in appropriate graphical/map format.

The feasibility of these two options is discussed below.

4.1.1 Option 1 — detailed modelling

The first task for Option 1 — the detailed modelling approach — would be to establish a programme of modelling based on a list of priority EPER substances. The highest priority would be to model the concentrations of the EPER substances most likely to cause harm to human health or the environment at concentrations arising from the emissions from EPER point sources. For many substances, objective concentration criteria have been determined to relate potential effects on human health or the environment to pollutant concentrations. Models can be used for these substances to relate the emissions from the EPER sources to environmental concentrations and hence to potential adverse environmental effects. For other substances, objective effects criteria have not been defined. Modelling may be helpful for specifying a research programme to establish environmental criteria for these substances, but an approximate estimate of environmental concentrations obtained by screening modelling will usually be sufficient for these purposes.

In order to justify the effort required for detailed modelling for a specific substance, it is necessary to have some evidence that suggests that the concentrations arising from point source emissions approach the concentration criteria in the environment. Environmental monitoring data may be available at the local level for the specific point source emission or similar sources. For example, considering the three test substances examined in Section 4.2, elevated hexachlorobenzene concentrations have been measured in surface waters; elevated benzene concentrations have been measured in the air near oil refineries; relatively high arsenic concentrations have been measured near to metal refining plant. Detailed modelling could be carried out at the local scale without screening in these cases.

Detailed regional scale modelling of EPER sources might be considered where the EPER emission makes up a large part of the known regional emission. Conversely detailed regional scale modelling of EPER sources would not be worthwhile where the EPER emission is relatively small. For example, detailed regional scale modelling for EPER sources of benzene would not be useful because the emissions from road traffic are much greater.

In many cases, the pollutant concentrations resulting from EPER point sources will be very small compared with the environmental health criteria. Carrying out detailed modelling without prior screening out of insignificant sources may be considered to be an ineffective use of resources. For example, the EPER database reports 227 arsenic emissions to air from individual sources in the range 20–1 600 kg y^{-1}. It is difficult to know which of these sources is likely to lead to concentrations approaching environmental criteria without some form of screening.

The second task would be to choose appropriate models to model the fate of the selected priority substances. The models described in the model evaluation study were categorised in terms of their dispersion medium (air, water, multimedia, etc.) and their scale (global, continental, regional or local). Most environmental models deal with a single environmental medium. Air dispersion models, for example, predict atmospheric concentrations resulting from the emissions to air. Single media models will be used where the release medium is the same as that associated with the selected environmental criterion. Multimedia models may be required where there is potential for significant transfer of the pollutant between media. However, the use of a multimedia model will usually entail a loss of detail in the individual media because computational compromises will be necessary. The extent to which pollutants will transfer between media depends on the release media (air, wastewater, surface water), the physical properties of the pollutant (e.g. solubility, vapour pressure, Henry's law constant, soil water partition coefficient etc.) and environmental conditions (e.g.

wind speed, land cover type). In some cases, it may be possible to assess the potential for cross-media transfer on the basis of expert judgement. For example, emissions of arsenic to the air will disperse in the atmosphere as particulate matter because arsenic is not volatile. The particulate arsenic will deposit onto the ground by dry deposition and wet deposition in precipitation. The deposited arsenic will not re-evaporate to any significant extent, but will be leached slowly from the soil by rainwater. The rate of leaching of the arsenic will be limited by its relatively low solubility so that it will accumulate in the top layers of soil until an equilibrium concentration is reached. The detailed modelling will therefore need to consider the dispersion in air of the particulate matter containing arsenic, its deposition to the ground and the leaching of arsenic from the soil. Screening models allow a more formal objective assessment of the potential for cross-media transfer to be made and place less reliance on expert judgment.

The highest environmental concentrations generally occur close to the emission source. Local scale models are therefore used to assess these impacts. Regional, continental and global models will be used where there are many point and diffuse sources contributing to pollutant concentrations. Nesting of local models within regional models may be required where the contribution from diffuse sources is similar to that from the individual point source. Screening models may be useful for assessing the relative contributions from individual point sources and regional sources.

Pollutant concentrations in the soil and sediments may increase gradually with time and only come to a steady state after many years, decades or centuries. Steady-state estimates of pollutant concentrations may therefore substantially overestimate environmental concentrations. Dynamic models are needed where there is a requirement to model the development of pollutant concentrations in the soil with time in detail. In some cases, useful approximations can be made with steady state models. For example, the rate of accumulation of a non-volatile substance such as arsenic in soil resulting from deposition from the atmosphere can be made using a steady-state atmospheric dispersion model and a simple dynamic soil mass balance. Decoupling of media calculations in this way can often lead to substantial reductions in computational effort.

The next stage of preparation for detailed modelling is to gather extensive datasets on emissions, chemical properties and speciation of emissions (including congener profiles of POPs, PAHs etc.) local and regional landscape parameters, meteorological information. It is therefore relevant to compare the availability of data for predicting the chemical density resulting from EPER releases with the data requirements for detailed modelling. EPER provides data on the total annual release to water or air of the chemicals it lists, released from large regulated facilities. Data on the basic physicochemical properties of most of these substances may be found readily in the chemical literature and properties databases. For a few substances such as dioxins and PAHs, however, emissions contain a large number of closely related forms that may show major differences in their environmental behaviour and biological properties. Currently, EPER contains no information on the detailed composition of such releases of these chemicals. Similarly, EPER contains no information on installation (61), environmental or landscape factors that determine the initial dispersion of the chemical following release, and hence its concentration in the local environment. Information on landscape, meteorology and hydrology that mainly determine the regional distribution of emissions is available in a number of European databases and could be used to assist detailed modelling. However, obtaining information on a local scale is likely to prove more challenging.

The definitive source of information on the individual releases listed in EPER is the installation operators. In most cases, information on local environmental concentrations of chemical releases and other details affecting dispersion in the environment will have been provided to the national regulatory authority for the purpose of obtaining an IPPC operating permit. If this information were available for chemical density assessment, there would be no need for further detailed modelling. However, industry is under no legal obligation to provide this and any supplementary information for purposes other than those of IPPC permitting and compliance, but may do so if requested on a voluntary basis. A possible approach for obtaining such local information is discussed in Option 2, below.

The computational resources required for detailed modelling depend on the spatial and temporal resolution of the model — the resources depend on

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(61) Other than geographical coordinates.

the distances between the receptor locations and the frequency at which model outputs are updated. Usually it is necessary to make some compromises between model spatial and temporal resolution. High spatial resolution models are required for local assessments close to point sources. Low spatial resolution models are often satisfactory for diffuse sources of emissions. High temporal resolution models are required where human health and environmental effects are related to short-term exposure. Low temporal resolution (annual average or seasonal average) models are appropriate where health effects are related to long-term exposure to chemicals.

The output from detailed models will require thorough evaluation if any reliance is to be placed on the models. This evaluation should include the comparison with monitoring data. Monitoring studies suitable for the evaluation of the models should be identified prior to carrying out detailed modelling. Detailed modelling may not be justified where there is insufficient monitoring data to verify the performance of the model for the chosen application.

It is concluded that there are a number of disadvantages associated with Option 1. These are as follows:

- Gathering detailed input data, running and interpreting a number of detailed models for a range of substances is expected to be very time consuming and therefore expensive.

- The choice of detailed model is not always clear-cut, especially when there are several comparable tools available that could be used, and could be open to challenge.

- Monitoring data for the thorough evaluation of the model may not be available. Without proper evaluation, it is uncertain that the results of the modelling will be more reliable than those from a screening assessment.

4.1.2 Option 2 — staged approach to modelling

The conclusions from the model evaluation reported in Section 3.6 showed that there are a range of well-established models available for screening and detailed modelling of the chemical concentrations in the environment from point source emission data, but because of the complexity of input data needed for detailed models, their application to all EPER substances would prove very resource intensive. Screening models, with their lower requirements for input data, may help to identify instances where further detailed modelling would be needed, hence allowing resources to be targeted more effectively. It is important to recognise that screening models are designed to be conservative and in practice screening models used for local assessments based on limited local information are often very conservative.

Site operators would, of course, be the definitive source of information on environmental concentrations of chemicals in the locality of emissions, or at least should have information that would allow such concentrations to be modelled with reasonable accuracy, but there is no obligation on companies to release this information. However, in many instances it is anticipated that local concentration data may already have been compiled for the purposes of obtaining an IPPC permit.

IPPC permit applications are public documents and in theory could be accessed to provide the additional information needed for chemical density prediction. In practice, however, we anticipate that obtaining information via this route would be difficult. In many cases, national regulators hold no database of the location of IPPC permit documents, this information commonly being held in paper copies at local or regional offices. Regulator may not necessarily be able to provide the resources needed to locate and provide copies of such information following requests for its provision and a personal visit may well be needed to gain access to the documents. Alternatively, making the results of the screening modelling publicly accessible may act as a spur to industry to provide information on local environmental concentrations on voluntary basis, as part of the EPER submission.

The staged approach to modelling that forms the basis of Option 2 is based on the EUSES screening model, with more detailed modelling being undertaken where screening indicates that relevant criteria may be exceeded on a regional (or greater) scale, or using information provided by industry where the screening method indicates that relevant local criteria may be exceeded. The strategy is outlined below. This approach was extensively discussed at the expert workshop on 16 August 2005. This section of the report presents the approach as originally developed and reviewed at the workshop. The work plan described in Section 4.3, however, takes account of the discussions at the workshop and the results of the model demonstration (reported in Section 4.2) to reflect the difficulties of presenting local environmental concentrations of chemicals without detailed site-specific release information.

The elements of the staged approach to chemical density modelling are listed below and summarised in the flow diagram shown in Figure 8:

1. A recognised screening model will be used to calculate local and regional environmental concentrations of chemicals from EPER emissions. The EUSES model, as the EU's established tool for chemical risk assessment will be used for this purpose. Default assumptions will be used in the first instance for the model. This will generally lead to highly conservative predictions.
2. The resulting predicted environmental concentrations will be compared with relevant environmental standards, or where these have not been established, with other relevant benchmarks or criteria. If these criteria are not exceeded, then there is the presumption that further refining of the estimated concentrations will not be required.
3. Where the relevant criteria are exceeded, then additional modelling with EUSES will be undertaken, with input data chosen to replace the default values and hence reduce the conservatism of the model. For example, discharge heights for emissions to air strongly affect local environmental concentrations. Sector specific stack height data will therefore be used to replace the default values.
4. The results will again be compared with the relevant criteria. If there are no exceedances then the modelling will be complete for this substance.
5. If predicted regional concentrations still exceed the relevant criteria, then other information will be sought to test the truth of this prediction. This information may take the form of regional monitoring or other modelling studies. If these fail to refute the conclusion that the relevant criteria may be exceeded on a regional scale, then detailed regional modelling would need to be undertaken.
6. If local environmental concentrations exceed the relevant criteria, then additional information will also be needed to refute or confirm this position. However, it is anticipated that in many instances the required information will already have been provided to the local regulatory authorities to support the installation's IPPC permit and will (at least theoretically) be available on the public record. This detailed information on local concentrations could then be used to overwrite the (conservative) screening model estimates.
7. For reasons outlined above, accessing installation IPPC permits for information on local concentrations of chemicals is expected to prove resource intensive. We suggest that after a suitable period of consultation, the current estimates of environmental concentrations are published on the Internet, together with full details of how the results were calculated to ensure full traceability and transparency. By publicising the screening model results on the Internet and with appropriate promotional measures to encourage buy-in, voluntary submission of the necessary data with the EPER returns may be encouraged. Although consistent with the principle of public access to environmental information enshrined in the Aarhus Convention, this approach may prove to be highly contentious, especially if the published results appear to be at variance with local regulatory limits.

This staged strategy to modelling has the following advantages over the alternative of detailed modelling of all EPER releases for predicting the chemical density of Europe:

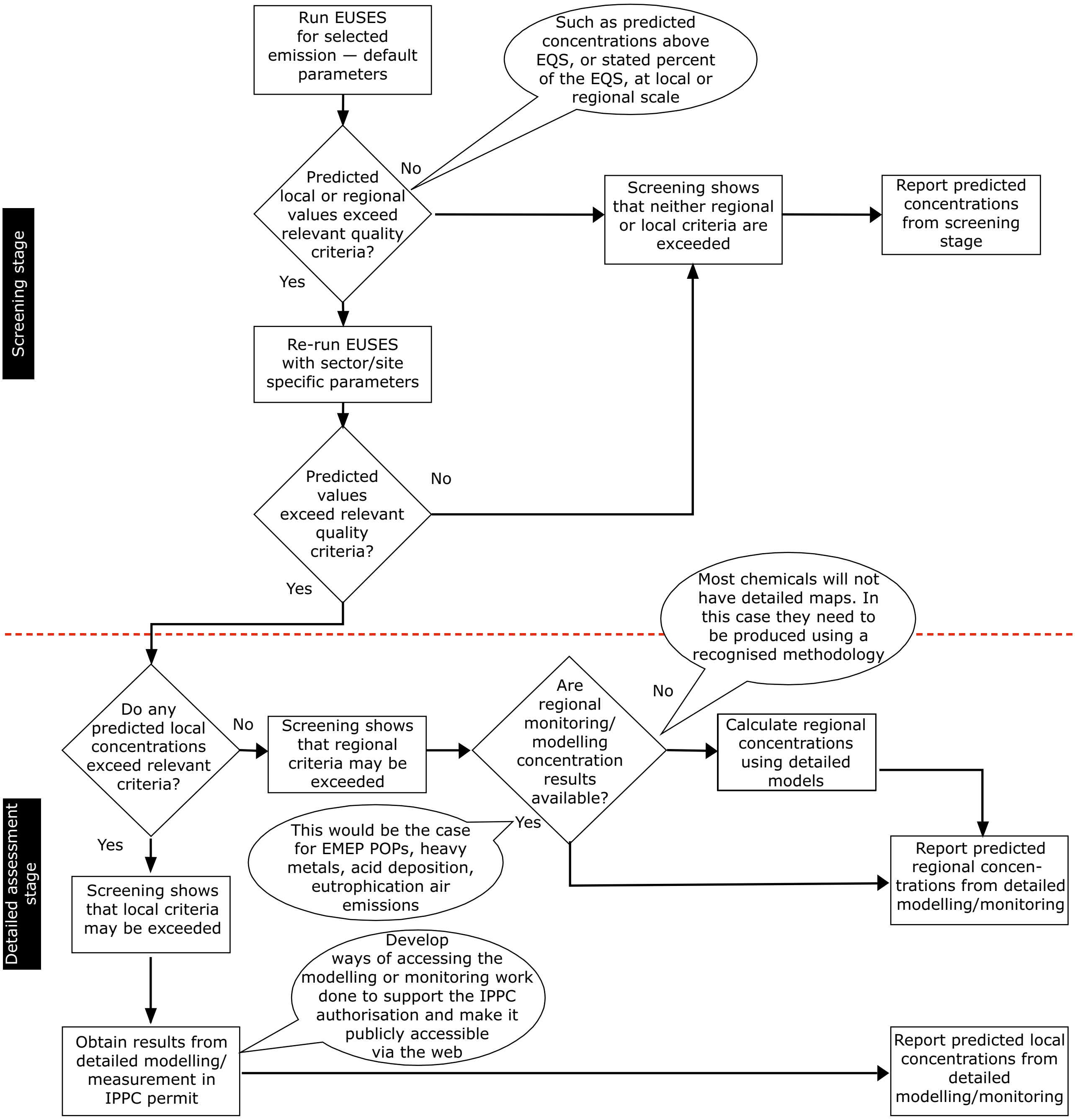
- Resource impacts will be much lower because of the use of an established screening model with extensive default information already provided. The resource required for running this model would be much less than that associated with a detailed model. Automating the loading of EPER data into a screening model can further reduce the resource input for model operation. There would be much less scope for automating this process with detailed modelling, where a variety of models would have to be used.

- The staged approach provides an interim assessment of the effects of the EPER releases. The interim assessment can be used to help clarify the objectives of more detailed studies.

- Efficiency is further improved because detailed regional modelling would only be required where the screening approach indicated exceedance of a relevant criterion, and if existing monitoring or modelling data are not already available.

- Industry would have an incentive to provide more detailed local information as an alternative to the screening model output. This would bear most strongly on installations producing the highest environmental concentrations, or concentrations that are closest to, or above, an environmental quality standard, consistent with cost effectiveness principles.

Figure 8 Stage approach to modelling chemical density (Option 2)



- Industry would have the option of providing monitoring data or the results of detailed modelling studies used to support the IPPC permit application. After undertaking the initial screening assessments, responsibility for the accuracy of the subsequently provided data would rest with industry.

- A flexible Internet tool for reporting concentration data would allow the output to be displayed in a variety of map configurations based on the detailed modelling provided by industry.

- Allowing industry to submit detailed information to replace the screening results would ensure that the system acts as an agent for stimulating environmental improvement.

Like other screening models, EUSES is specifically designed for predicting the concentration of chemicals emitted into the environment: it is not suitable for chemicals for which the major concerns are dependent on some other product formed as a result of the primary release. Examples of these secondary pollutant effects are acidification and eutrophication of surface water and soil via air pollution and the formation of ozone and other oxidants. Fortunately, extensive modelling and monitoring programmes are underway under the auspices of the CLTAP that provide regional information on acid deposition and photochemical oxidants so that further detailed modelling for the effects for EPER releases will not be required.

The staged approach is consistent with the tiered approach to modelling endorsed in the OECD technical guidance document [17] for the related challenge of predicting persistence and potential for long-range transport of chemicals, with each tier representing and increasing level of complexity. The OECD goes on to note that:

> *…accuracy of a model represents its capacity to give results that tend to centre on the true answer (even if it is not precise). Increasing model complexity generally aims at increasing the accuracy of the results, but also leads to a need for a greater amount of more accurate input data as well as higher levels of user expertise. The choice of model should always be driven by the objectives of the user as well as his constraints in terms of data and resource availability.*

We conclude that this approach will provide a cost-effective basis for predicting the chemical density of Europe. The next section of the report demonstrates how EUSES can be used with EPER data releases for three test substances, as part of the staged modelling approach outlined above.

4.2 Demonstration of the staged approach to modelling chemical density

This section corresponds with Task 6 in the technical specification (Appendix 1), which sets out the following requirements:

- Run one or more selected readily available models for one or more test substances by using the reported release data in the EPER database. In selection of the test substances consider the availability of monitoring data on the compounds as a key requirement.

- Map the concentrations.

- Identify hot spots of predicted high chemicals concentrations.

- Assess the usefulness of the EPER data format for this purpose. For substances already covered by EMEP discuss the added value of using EPER data for high and smaller resolution assessments. Will EPER data increase the usefulness of existing models on (pan) European, regional or local level?

- Compare predicted levels with actual monitoring data on concentrations, if available.

The approach advocated in the previous section indicated that a staged approach to the assessment of the fate of chemicals in the environment was most likely to be cost-effective (i.e. Option 2). It identified the EUSES model as an appropriate tool for the screening of the impacts of point sources listed in the EPER database. This section of the report demonstrates how EUSES can be used to predict the fate in the environment of three chemicals released from point sources listed EPER. The chemicals selected were:

- hexachlorobenzene, an example of a persistent organic pollutant (POP);

- benzene, an example of a volatile organic compound;

- arsenic, an example of a heavy metal.

These chemicals were selected to represent the range of potential application of the EUSES model. The latest publicly-available version of EUSES at the time of writing was used. This is version 2.0.3.

The concentrations of the selected substances in air are monitored throughout Europe and the data are collated in the EMEP database (62). EMEP produced a summary report for heavy metals and POP measurements in 2002 (63). An EMEP report summarised measurements of hexachlorobenzene concentrations in the environment (64). Further monitoring data for benzene and hexachlorobenzene are listed in the IUCLID database (65). It was therefore concluded that there is sufficient monitoring data available for these substances to meet the selection criterion set out in the technical specification.

The following paragraphs describe the method used for preparing input files for the EUSES model and the preparation of maps showing the predicted environmental concentrations (PECs) at various spatial scales. We then describe the results of the modelling demonstration based on input data for each of the three test chemicals. The remaining sub-sections show how screening model outputs may be overwritten as better information becomes available, considers the usefulness of the EPER data and finally describes how the requirements for more detailed modelling may be defined from the outcome of the screening stage.

4.2.1 *Preparation of model input files*

The EPER database provides various data tables. These include the following:

- Emission: a list of reported emissions. The data table identifies the facility from which emissions take place, the emission type (air, direct to water, indirect to water), the type of emission estimate (measured, calculated or estimated), the pollutant and the quantity emitted (in kg/year) for each emission.

- Facility: a list of emitting facilities. The data table identifies the company that operates the facility, the address and the latitude and longitude of each facility.

A Visual Basic in Excel® script was developed and used to extract emissions data from the EPER database for specified pollutants. The script identified where more than one emission to the same media type was reported for the same facility and aggregated the reported emissions. The script also identified other EPER emission sources for the specified pollutant that are located within a 200 x 200 km region centred on each emitting facility: the emissions were aggregated to provide a 'regional EPER emission'. A 'continental EPER emission' was also calculated as the sum of all EPER emissions of the pollutant for each media type, excluding the regional EPER emission.

The process is shown schematically in Figure 9. Consider a facility located at A. All the emissions from the facility at A into the same medium are added together to provide a local emission. A region extending 100 km in the directions north-south and east-west is defined for facility A. In other words, A is centred within a 200 x 200 km region. All the EPER emissions into each medium from facilities in the region, excluding A itself, are added together to give the 'regional EPER emission'. In Figure 9, the emissions from facilities B, C and D are added together. The EPER emissions outside the region are also added together (in this case from facilities E, F and G) to give the 'continental EPER emission'. Local, regional and continental emissions are defined in this way for each facility within the EPER database.

As an alternative option, a 'regional background emission' and a 'continental background emission' were calculated based on the officially reported emissions to air for each European country (66). The regional background emission for the 200 x 200 km area centred on each emitting facility was calculated from the national total on a pro-rata basis by area.

EUSES 2.0.3 provides the facility to import and export text data files (*.EXF). The Visual Basic script reads in a template EUSES exchange file and modifies it to provide an updated input file for each of the facilities emitting the specified pollutant. The EUSES export files contain details of local, regional and continental emissions and physical, chemical and biological property data for the specified pollutants. Pollutant specific property data was taken from the risk assessment reports carried out under Council Regulation 793/93, the IUCLID database (67), EMEP reports (e.g. Vulykh and Putilina

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(62) http://www.nilu.no/projects/ccc/emepdata.html.

(63) Aas and Breivik (2004).

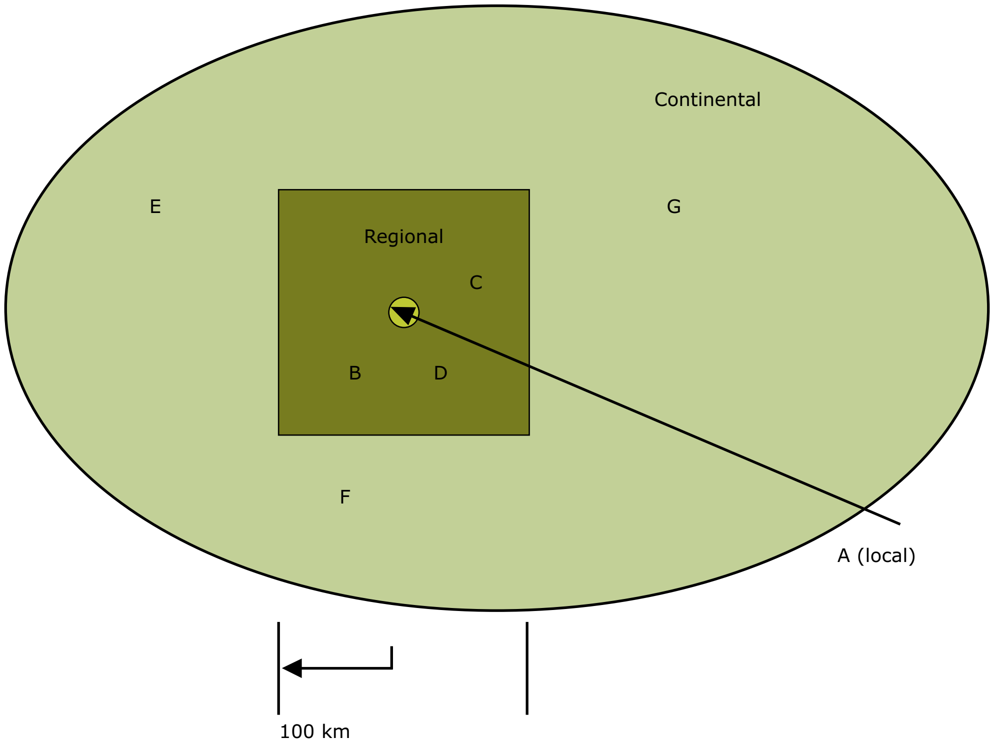
(64) N. Vulykh and V. Putilina. Hexachlorobenzene properties, emissions and content in the environment. EMEP/MSC-E Technical Note 6/2000, June 2000.

(65) http://ecb.jrc.it/ESIS/.

(66) http://webdab.emep.int/.

(67) http://ecb.jrc.it/ESIS/.

Figure 9 Schematic diagram of the local, regional and continental emissions



(2000) for hexachlorobenzene ([64], p.74) or the US EPA Human Health Assessment Risk Protocol ([68])).

EUSES 2.0.3 can be run for several facilities in batch mode. The Visual Basic script prepares a batch file to enable EUSES to be run for each of the emitting facilities.

For this feasibility study, we have used the default environmental data contained within the EUSES model. However, we have considered the potential for using other environmental data. Region-specific environmental data that could be used by EUSES includes:

- Temperature
- Population density of the region
- Average wind speed
- River flow rates
- Annual precipitation
- Area fraction of freshwater in the region
- Area fraction of natural soil in the region
- Area fraction of agricultural soil in the region
- Area fraction of urban or industrial soil in the region
- Area fraction of sea water in the region

This information could be extracted from climate databases (e.g. http://www.cru.uea.ac.uk/cru/data/hrg.htm), land use databases (e.g Corine) or river catchment databases (e.g. ERICA) by reference to the latitude and longitude coordinates of the EPER source or to the relevant country. Examples of relevant sources of this information are shown in Table 19. The required development to the EUSES data input script would be straightforward.

4.2.2 *Preparation of maps*

A second script was prepared in Visual Basic for Excel to prepare simple maps of pollutant concentrations. The script takes the EUSES exchange file outputs for facilities emitting the selected pollutant and reads the pollutant concentration output. The user selects the appropriate concentration outputs according to the parameter identifiers used in EUSES: for example, the contribution of each facility to local air concentrations is identified as 'PA LocalAir'. The script then converts the latitude and longitude of each facility to EMEP 150 km coordinates and plots the location on a map of Europe. In the examples that follow, the size, shape and colour of the marker is used to denote the magnitude of the concentration value.

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(68) http://www.epa.gov/earth1r6/6pd/rcra_c/protocol/protocol.htm.

Table 19 Information sources for chemical modelling

Database	Address	Comments
Screening Information Datasets for high production chemicals (SIDS)	http://www.chem.unep.ch/irptc/sids/OECDSIDS/sidspub.html	OECD initial risk assessment documents
Concise International Chemical assessment Documents — CICADs	http://www.who.int/ipcs/publications/cicad/en/index.html	CICADs summarises information needed for chemical risk assessment. They are produced under the WHO International Programme on Chemical Safety
INERIS Chemical Substances Portal	http://chimie.ineris.fr/en/lien/basededonnees/environnementale/recherche/search1_1.php	Environmental database of 573 chemicals
IUCLID (International Uniform Chemical Information Database)	http://ecb.jrc.it/existing-chemicals/	The database includes all data sets submitted by industry following council regulations (EEC) 793/93 on the 'evaluation and control of risks of existing substances.' The regulation mandates that industry submit all readily available data on High Production Volume Chemicals (HPVCs)
TOXNET	http://toxnet.nlm.nih.gov/	TOXNET is run by the US National Library of Medicine. It is a cluster of databases on hazardous chemicals, including: Hazardous Substances Data Bank (HSDB), Integrated Risk Information System (IRIS) and International Toxicity Estimates for Risk (ITER)
Agency for Toxic Substances and Disease Registry — ATSDR	http://www.atsdr.cdc.gov/hazdat.html	Haz Dat — ATSDR's Hazardous Substance Release and Health Effects Database
International Union of Pure and Applied Chemistry — IUPAC.	http://www.iupac.org/dhtml_home.html	Links to databases of environmental chemistry
European Water Quality Database — Waterbase	http://dataservice.eea.eu.int/dataservice/available2.asp?type=findkeyword&theme=waterbase	European Environment Agency's database of water quality, river flows and discharge. Includes rivers, lakes, groundwater and coastal and transitional waters
European Air quality database — AirBase	http://air-climate.eionet.eu.int/databases/airbase/	Air quality data and metadata for Europe
European landcover database — Corine	http://dataservice.eea.eu.int/dataservice/metadetails.asp?id=678	Landcover database for Europe
Catchment Characterisation and Modelling database — CCM	http://agrienv.jrc.it/activities/catchments/	European-wide river and catchment database for future use in environmental modelling activities. The database corresponds to a mapping scale of roughly 1:250 000 to 1:500 000, depending on the region
European Rivers and Catchments database — ERICA	http://dataservice.eea.eu.int/dataservice/metadetails.asp?id=235	The European rivers and catchments database (ERICA Version 1998) at scale 1:1 000 000 contains over 1 500 catchments to river confluences for the largest rivers in EEA member states
European Nature Information System — EUNIS	http://eunis.eea.eu.int/index.jsp	EUNIS contains: Data on Species, Habitats and Sites compiled in the framework of NATURA2000
Towards a European Chemicals Information System: a survey on reported monitoring activities of chemicals in Europe	http://eea.eionet.eu.int/Public/irc/eionet-circle/chemicals/library?l=/chemical_inventory&vm=detailed&sb=Title	Report and database prepared for the EEA on chemical monitoring activities being undertaken in Europe
International Commission for the Protection of the Rhine (Internationalen Kommission zum Schutz des Rheins — IKSR)	http://www.iksr.org/	Information on water quality measures, inorganic and organic pollutants and physico-chemical properties of the River Rhine at various monitoring stations
Estimation of willingness-to-pay and cost-benefit analysis for reducing heavy metals occurrence in Europe (ESPREME)	http://espreme.ier.uni-stuttgart.de/	Initial database of European heavy metal emissions in year 2000

The range of possible concentration outputs from EUSES is large. Table 20 summarises the main outputs at the local, regional, continental and global (arctic, tropical and temperate regions). The output presented as part of this feasibility study has been limited to the consideration of air, water or soil concentrations at the local, regional or continental scales. However, it would be possible to present other outputs in the same way. For example, it would be possible to present the predicted contribution from each EPER source to arctic sediment concentrations.

It was convenient to use Excel Visual Basic to prepare maps for this feasibility study. The use of GIS systems such as ArcView or MapInfo would allow a more sophisticated presentation of the results. Possible enhancements to the display could include:

- accurate scaling of the markers in proportion to the calculated concentrations;
- the use of a regular regional grid rather than the facility-orientated regions defined in the current study. This would prevent overlapping of regions where facilities are close together.

4.2.3 Hexachlorobenzene assessment

The EPER database lists three emissions of hexachlorobenzene from three separate facilities. All the emissions in the database were direct to water and had been measured rather than

Table 20 Output concentration data available from EUSES

Media	Geographical scale					
	Local	Regional	Continental	Arctic	Tropical	Temperate
Air	3	3	3	3	3	3
Surface water	3	3	3	3	3	3
Sea water	3	3	3			
Freshwater	3	3	3			
Agricultural soil	3	3	3			
Grassland soil	3					
Natural soil		3	3			
Industrial soil		3	3			
Soil				3	3	3
Freshwater sediment	3	3	3			
Marine sediment	3	3	3			
Sediment				3	3	3
Soil pore water	3	3	3			
Groundwater	3					
Fish	3	3				
Plants	3	3				
Drinking water	3	3				
Meat	3	3				
Milk	3	3				
Freshwater fish	A	A				
Sea water fish	A	A				
Fish-eating top predators	A	A				
Earthworms	A	A				

Note: A = combined regional/local prediction for the assessment of secondary poisoning.

estimated or calculated. The facilities reporting hexachlorobenzene emissions were in France, Germany and Belgium and were in the range 2–6 kg/year (69).

Hexachlorobenzene is released into the environment as an unintentional product from the chemical and metal industries. It was formerly manufactured for use as an agricultural fungicide, but its marketing and use as a plant protection product in the EU was banned in 1988. The substance has a number of adverse health and environmental impacts, for example, it has the following Risk Phrases: R45 — 'May cause cancer'; R48/25 — 'Toxic: danger of serious danger to health by prolonged exposure if swallowed' and R50/53 — 'Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment'. The substance is not listed in a priority list (as foreseen under Council Regulation (EEC) No 793/93 on the evaluation and control of the risks of existing substances) nor is there a risk assessment available under this legislation. Further information on the safety issues, environmental fate, ecotoxicity and toxicity of hexachlorobenzene is available from the European chemical Substances Information System (ESIS) (70).

Table 21 Official estimates of hexachlorobenzene emissions, 2003

Country	Emission, kg/year
Austria	0.47
Belgium	61.3
Germany	Not available
Denmark	Not available
Spain	6 145
Finland	0.46
France	1 762
Greece	0
Ireland	0.04
Italy	0
Luxembourg	0
Netherlands	0
Portugal	0
Sweden	Not available
United Kingdom	302
Total	**8 271.27**

Official estimates of national emissions obtained from the EMEP Internet WebDab site were used to estimate regional and continental emissions to air and these are shown in Table 21. It is notable that emission estimates from various countries differ by orders of magnitude: we have not investigated whether this indicates that there are substantially different emissions in each country or whether emission-reporting standards differ between countries.

Table 22 shows the physical and chemical properties of hexachlorobenzene used for the model runs. Other properties were calculated in the EUSES model using Quantitative Structure Activity Relationships (QSARs) for hydrophobic substances.

Predicted concentrations of hexachlorobenzene were calculated for air and surface water and the results are presented below. It should be remembered that because hexachlorobenzene has appreciable volatility, emissions to water will also contribute to concentrations in the air.

Dealing first with the results for concentrations in air, Figure 10 shows the predicted local concentration of hexachlorobenzene in air resulting from the sources listed in EPER. The screening model predicts that EPER sources make a substantial contribution (up to 632 pg m^{-3}) to local air concentrations within 100 m of the source.

The contribution from all EPER sources to the regional concentrations (shown in Figure 11) is relatively small (less than 0.4 pg m^{-3}). The predicted maximum regional background concentration from all sources except EPER sources is approximately 110 pg m^{-3} (Figure 12). The local predicted environmental concentration (PEC) due to all sources is the sum of the regional background and the local contribution from EPER sources, i.e. a maximum concentration of $110 + 632 \approx 740$ pg m^{-3} (Figure 13).

Aas and Breivek (2004) (71) present monitoring data for background sites in the far north of Europe for 2002. The annual average concentrations are shown in Table 23.

Vulykh and Putilina (2000) (64, p.74) present older data for more urban regions. Mean concentrations

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(69) The database used for this assessment was downloaded from the EPER website in April 2005. We note that the current website database (dated 27 May 2005) contains an additional fourth emission of 1.88 kg/year of hexachlorobenzene, also directly to water, from a facility in the United Kingdom. This facility has not been included in this assessment.

(70) http://ecb.jrc.it/esis/esis.php?PGM=ein.

(71) Aas, W. and Breivik, K. *Heavy metal and POP measurements 2002*. EMEP/CCC report 7/2004.

Table 22 Properties of hexachlorobenzene used in the assessment

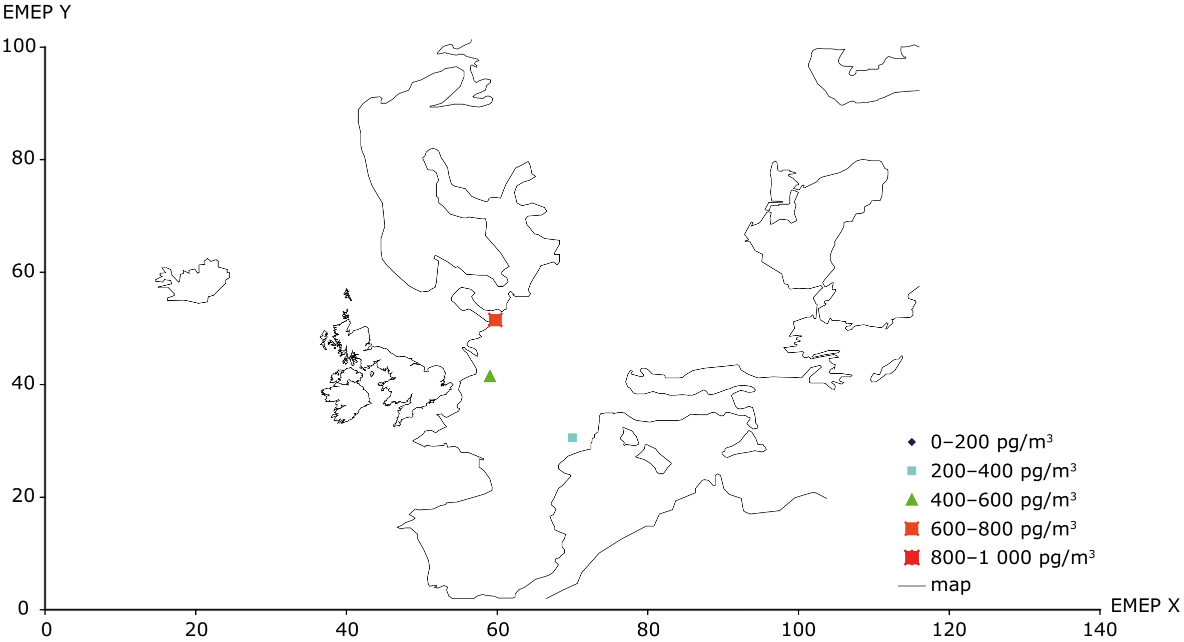
Property	Value
Molecular weight	284.8
Melting point, °C	231
Boiling point, °C	309
Vapour pressure, Pa	0.0011
Temperature of vapour pressure measurement, °C	20
log K_{ow}	5.5
Solubility (mg/l)	0.01
Temperature of solubility measurement, °C	20
Degradation rate in air, day^{-1}	0.0009
Henry's law constant, Pa m^3 mol^{-1}	76

for sites in Germany, France and the Czech Republic are shown in Table 24. The data for Ulm and Hamburg are referred to in the IUCLID database as being relevant to a contaminated site.

It is not possible to make a direct comparison between the measured concentrations and the concentrations predicted by EUSES because modelled and measured estimates were not made at the same locations. Nevertheless, it appears that EUSES predicts HCB concentrations in air within an order of magnitude.

Figure 14 shows the predicted local environmental concentration in surface waters, based on default values for input parameters in EUSES. The highest

Figure 10 Predicted environmental concentration of hexachlorobenzene in air — EPER contribution to local concentration



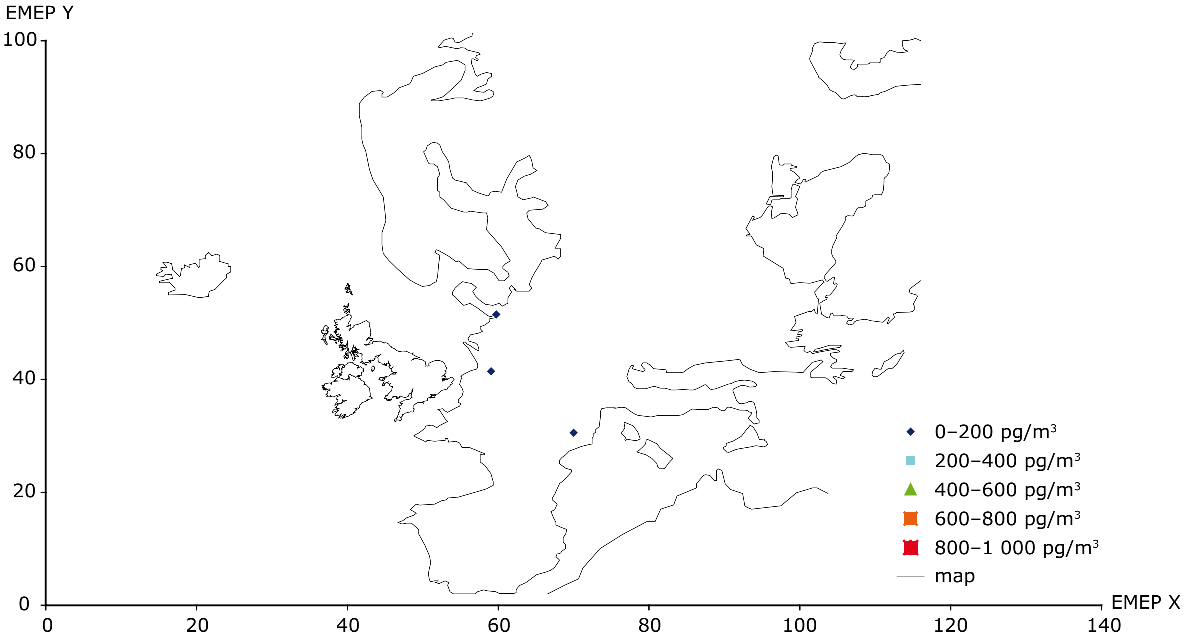
Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicates the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

predicted environmental concentration (PEC) was 124 ng l^{-1}. The regional background concentration is small (< 0.02 ng l^{-1}). The IUCLID database reports concentration measurements in surface waters at a contaminated site of 2–30 ng l^{-1} in the River Rhine in 1985–1989 and 6–50 ng l^{-1} in the River Elbe in 1980–1989. Again, it is not possible to make a direct comparison between the measured concentrations and the concentrations predicted by EUSES. Nevertheless, it appears that EUSES predicts hexachlorobenzene concentrations in surface waters at a contaminated site within an order of magnitude.

Council Directive 88/347/EEC sets a quality objective for hexachlorobenzene of 30 ng l^{-1} for inland and coastal waters. It is possible that the PEC will exceed the water quality standard near some of the EPER sources. More detailed assessment of concentrations in surface waters may be necessary in this case.

As a result of this assessment, we can draw the following **conclusions** for hexachlorobenzene:

Figure 11 Predicted environmental concentration of hexachlorobenzene in air — EPER contribution to regional concentration

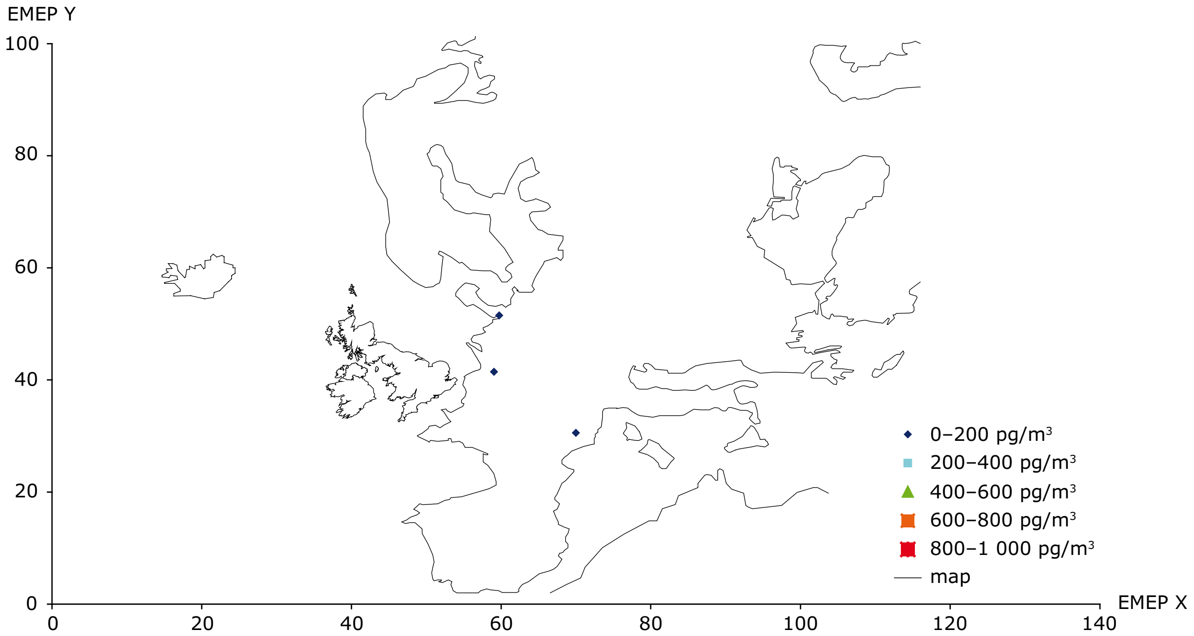


Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicates the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

Table 23 Hexachlorobenzene concentrations in air in northern Europe

Site	Country	Concentration, pg m^{-3}
Pallas	Finland	38
Storhodi	Iceland	3.7
Zeppelin, Spizbergen	Norway	56
Lista	Norway	57

Figure 12 Predicted environmental concentration of hexachlorobenzene in air — regional background concentration



Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicate the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

Table 24 Indicative hexachlorobenzene concentrations in air in urban Europe

Site	Country	Period	Concentration, pg m^{-3}
Ulm	Germany	Winter 1987	250
Hamburg	Germany	1986–1987	600
Strasbourg	France	April–May 1993	483
near Colmar	France	April–May 1993	317
Kosetice	Czech Republic	July–December 1994	208
Kosetice	Czech Republic	November 1996–December 1998	181

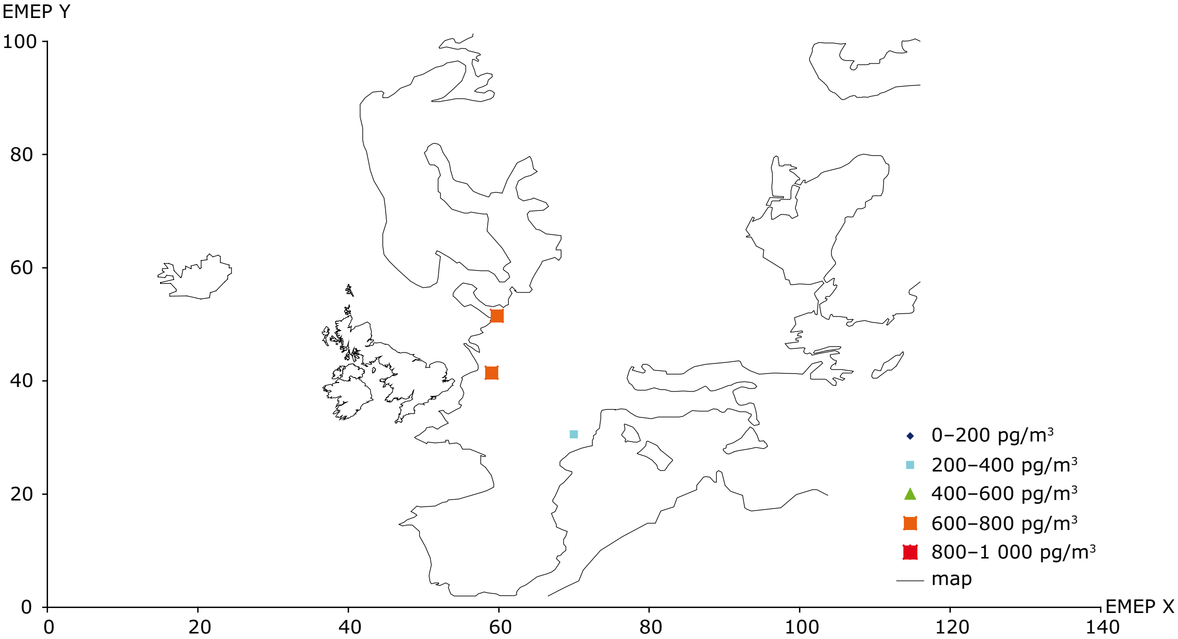
- There are few sources of hexachlorobenzene listed in the EPER database.

- Official national estimates of hexachlorobenzene included in the EMEP database are not complete.

- The EUSES model provides predictions of regional hexachlorobenzene concentrations in air and surface waters that are within an order of magnitude of measured concentrations.

- Predicted environmental concentrations in surface waters may exceed quality standards close to EPER data sources according to the results of initial modelling with EUSES based on default input parameters: further local modelling with EUSES of emissions to water may be required using site-specific information to determine if a more detailed (and resource intensive) assessment with a spatially-resolved model is required.

Figure 13 Predicted environmental concentration of hexachlorobenzene in air — Local PEC



Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicate the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

- Maps produced from EUSES model run outputs clearly show the location of potential hot spots and the predicted pollutant concentrations.

4.2.4 Benzene assessment

Benzene is used as a reagent in the production of a wide variety of chemical substances, having applications such as: dyes, detergents, coatings, plastics, fibres, pesticides, adhesives and coatings, lubricating oil additives, dry cleaning fluids, paint and production of some types of rubber. Benzene is also found in crude oil, petrol and cigarette smoke. Benzene is released to the environment as a result of vehicle exhaust emissions, evaporation of petrol during vehicle fuelling and from fuel tanks, stack emissions from fuel combustion and as fugitive emissions from its manufacture and use in the chemical industry.

Benzene is harmful to human health. The substance is classified under several Risk and Safety Phrases. In relation to environmental exposure of humans, the most important of these would appear to be R45 — 'May cause cancer' and R46 — 'May cause heritable genetic damage'. Benzene is on the 1st list of Priority Chemicals under Council Regulation (EEC) 793/93: a draft risk assessment prepared under this regulation is available, dealing with environmental risks (May 2002) and health risks (March 2003) (72). Benzene is also categorised and regulated as a volatile organic compound (VOC) and as such emissions can contribute to the formation of potentially harmful concentrations of ozone in the lower atmosphere. Further information on safety issues, ecotoxicity, toxicity of benzene is available from ESIS. Benzene has been considered in this feasibility study in order to demonstrate the application of the method to an example of a VOC. The results of the assessment are intended only as an illustration of the method. Those wishing to obtain detailed information on risks to human health or the environment should refer to the EC Risk Assessment.

The EPER database listed 217 emissions of benzene. All the listed emissions were released to air. The quantities emitted from each source were in the

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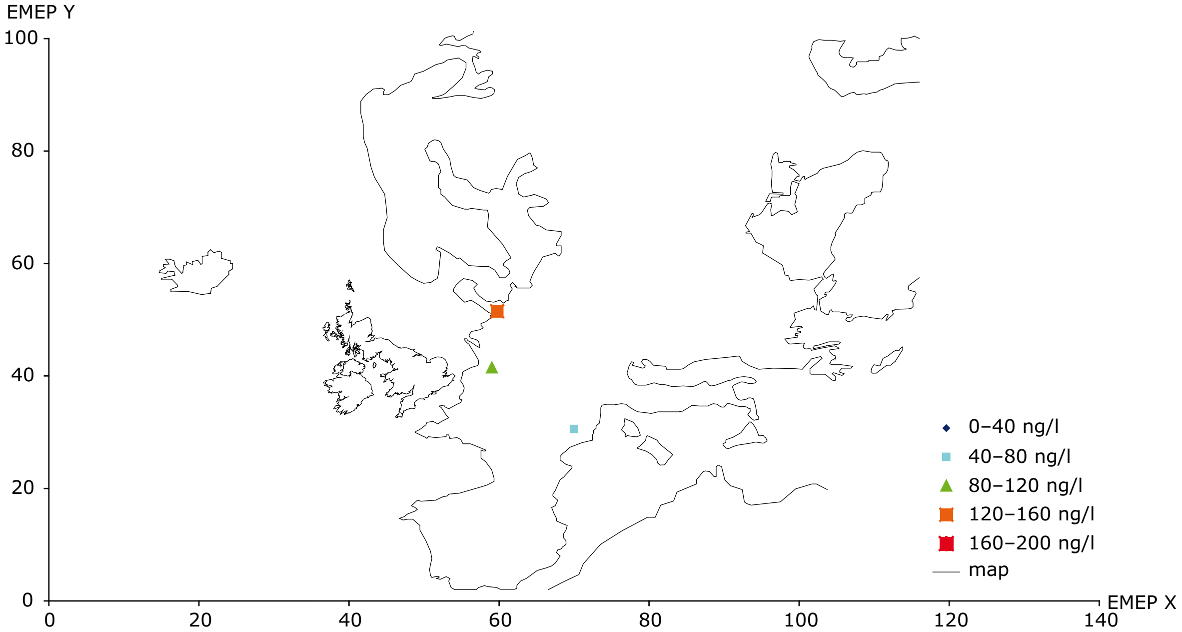
(72) Risk Assessment — Benzene (Environment Part, May 2002, and Human Health part, March 2003) http://ecb.jrc.it/esis/esis.php?PGM=ein.

Figure 14 Predicted surface water concentrations of hexachlorobenzene



Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicate the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

range 115 kg to 295 000 kg per annum with a total EPER emission of 3 961 275 kg per annum. Of the reported emissions, 62 were measured, 78 were estimated and 77 were calculated.

Benzene emissions generally have been decreasing steadily since 1990. For example, emissions in the United Kingdom are now about 20 % of 1990 levels, according to the National Atmospheric Emission Inventory (73). These decreases are primarily due to the introduction in 1991 of cars equipped with catalytic converters, although emissions from the domestic and industrial sectors are also falling. The emissions of benzene from EPER sources are generally small compared with emissions from other sources. EPER sources accounted for about 12 % of the United Kingdom's 14 600 000 kg of benzene emitted in 2001, the largest source of which was car exhaust emissions. Benzene emissions are not reported in the UNECE/EMEP (United Nations Economic Commission for Europe/Co-operative programme for monitoring and evaluation of long-range transmission of air pollutants in Europe) emission database. We are not aware of any other consistent databases of European national or regional emissions totals for benzene.

The emissions from benzene production and processing have decreased markedly since the EU Risk Assessment was carried out. The Risk Assessment considered the emissions to air from 48 facilities. The emissions data for some of these facilities relates to 1995 or earlier. The total emission direct to air from the 48 facilities was 45 503 kg per day. This is substantially more than the reported total emission for 2001 from EPER sources of 10 853 kg per day. The maximum daily emission direct to air from an individual facility considered in the EU Risk Assessment was 17 867 kg per day: the maximum emission from any individual EPER emission source was 808 kg per day. The reductions in emissions are the result of the substantial efforts taken by industry to this end.

The EPER database also includes emissions of 'BTEX' (a mixture of benzene, toluene ethylbenzene and xylenes, of unspecified proportions) to water. No attempt has been made in this feasibility study

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(73) http://www.naei.org.uk/emissions/emissions_2002/summary_tables.php?action=unece&page_name=BZ02.html.

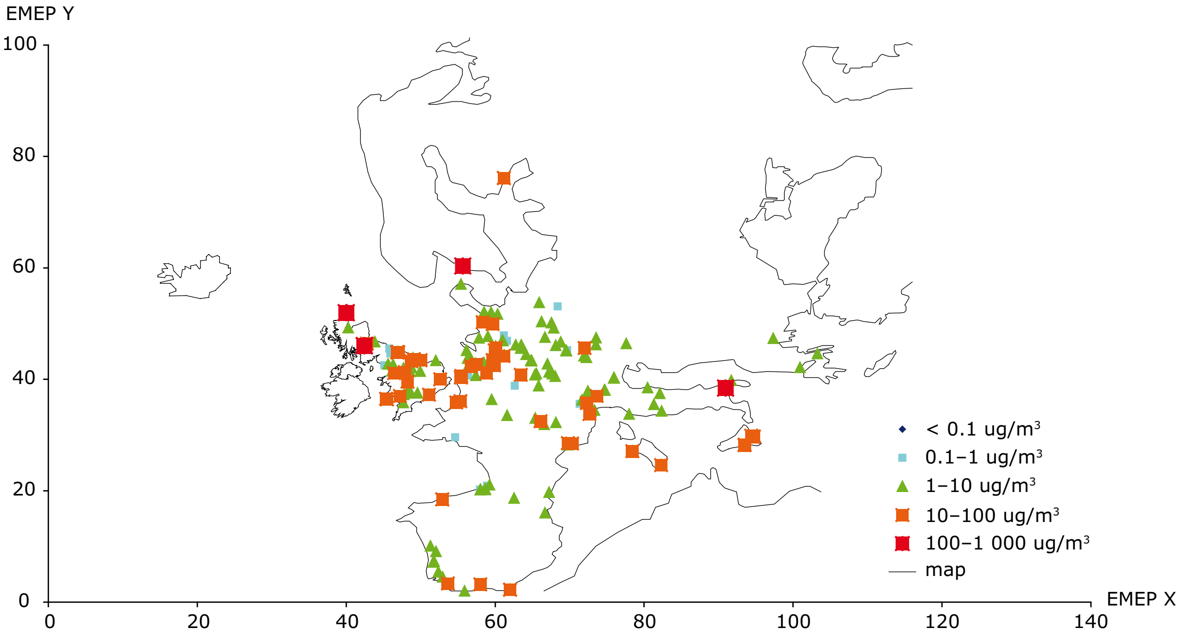
to estimate the proportions of benzene in each of the reported BTEX emissions: the assessment does not take these emissions into account (74).

Table 25 shows the physical and chemical properties of benzene used for the model runs. Other properties were calculated in the EUSES model using Quantitative Structure Activity Relationships (QSARs) for non-hydrophobic substances.

Figure 15 shows the contribution from EPER sources to local predicted environmental concentration of benzene in air, based on initial modelling with EUSES and default input value parameters. The maximum predicted contribution to local benzene concentrations was 225 µg m^{-3}. This is large compared to the predicted regional background concentration: for example, the regional background concentration in the United Kingdom (75) was predicted to be 0.15 µg m^{-3}. The contribution from EPER sources to regional background concentrations was also small (typically 0.02 µg m^{-3} or less).

Parties to the Convention on Long-range Transboundary Air Pollution perform monitoring of benzene at regional monitoring sites across Europe. Table 26 shows the measured benzene concentrations at these sites during 2002. Table 27 shows measured annual average concentrations measured in the United Kingdom as part of the automatic urban and rural monitoring network (76). Generally the regional background concentrations predicted by EUSES are rather smaller than the measured concentrations in urban and rural

Figure 15 EPER contribution to local predicted environmental concentrations of benzene in air



Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicate the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

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(74) Assuming that all of the BTEX released was in the form of benzene, then total EU release to water in this form would amount to a maximum of just over 8 % of the emissions to air.

(75) The draft EU Risk Assessment for benzene cites a range of 1.5 to 4.4 µg m^{-3} of benzene rural air. However, as the risk assessment was based on measurements made during the 1990s when emissions were considerably higher than today, the current UK figure provides the more relevant comparison.

(76) http://www.airquality.co.uk/archive/data_and_statistics.php.

Table 25 Properties of benzene used in the assessment

Property	Value
Molecular weight	78
Melting point, °C	5.5
Boiling point, °C	80.1
Vapour pressure, Pa	10 000
Temperature of vapour pressure measurement, °C	20
log K_{ow}	2.13
Solubility (mg l^{-1})	1 800
Temperature of solubility measurement, °C	25
Degradation rate in air, day^{-1}	0.124
Henry's law constant, Pa m^3 mol^{-1}	550

areas. The predicted contributions from many EPER sources to local concentrations are rather larger than measured concentrations at urban and rural locations. The EUSES predictions of local concentrations are intended to be conservative and so the dispersion model predicts ground level concentrations at a distance of 100 m from the source assuming the whole of the emission is released through a 10 m high stack without buoyancy or momentum.

The predicted concentrations can be compared with the limit value of 5 µg m^{-3} as an annual mean set in the Second Air Quality Daughter Directive to be achieved by 2010. The EUSES model predicts that the limit value could be exceeded close to many of the EPER source locations. However, it is important to remember that this assessment is based on the default assumption concerning local release and dispersion, which will result in highly conservative estimates of the local PEC, and so measured concentrations at many of these sites may be expected to be below the limit value. These initial screening results would therefore indicate that more detailed assessment of local air quality would be required for many of these EPER sources. To confirm this conclusion, further EUSES modelling should be undertaken, using input data more representative of the processes leading to the emissions than are reflected in the default input parameters used for the initial screening. The assessment for arsenic emissions to air (described in Section 4.2.6) clearly shows how predicted local concentrations may be significantly reduced as further information on stack height, plume discharge characteristics and local dispersion is used to overwrite the default EUSES input data and so reduce the level of conservatism in the results. If the results of further screening with EUSES using this site-specific information for benzene releases still show exceedence of relevant criteria, then this would signal the need for further detailed spatially resolved local modelling and investigation.

The more detailed assessment should take account of the characteristics of the discharge (including the number and location of emission points, stack heights and diameters, discharge temperatures and velocities), meteorological conditions during release and the presence of topographical features such as buildings and hills that might influence pollutant dispersion. Much of this key information is not publicly available, so making the assessment of local concentrations by bodies other than the site operators, local regulators or their agents with access to the required information highly problematical.

The predicted contribution from EPER sources to surface water concentrations is very small (typically less than 2 ng/l — results not shown). This may be compared with average surface water concentrations reported in the IUPAC database of 7.05 µg /l for 80 rivers and estuaries in the United Kingdom in 1988/1989 (cf 30 µg /l UK legislation).

The following **conclusions** are drawn from the assessment for benzene:

- There are a large number of benzene emission sources to air identified in the EPER database.
- Benzene emissions are not reported in the EMEP database.

Table 26 Measured benzene concentrations in air (CLRTAP)

Site code	Site name	Concentration, μg m^{-3}
CH0005R	Rigi	0.68
CZ0003R	Kosetice	0.96
CZ0099R		1.40
DE0002R	Waldof	0.82
DE0005R	Brotjacklreigel	0.63
DE0008R	Schmucke	0.70
DE0009R	Zingst	0.73
DE0043R		0.70
ES0009R	Campisabalos	1.07
FI0009R	Uto	0.54
FR0008R	Dunon	0.65
FR0013R	Payrasse Vieille	0.48
FR0015R	La Tardiere	0.60
SK0006R	Starina	0.96

Table 27: Urban benzene concentrations in the United Kingdom in 2004 (77)

Site name	Annual mean concentration, μg m^{-3}
Cardiff Centre	0.85
Glasgow Kerbside	1.41
Harwell	0.6 (2003)
London Eltham	0.76
London Marylebone Road (kerbside)	2.75

- The contribution from EPER sources to regional background benzene concentrations in air and surface water is small.
- The EUSES model underestimated regional background concentrations in water: however, this unsurprising because neither the EPER database nor the UK national atmospheric emission inventory contains entries of emissions to water, and as mentioned in the earlier discussion of benzene release data, the contribution of benzene in releases to water of the mixture listed in EPER as 'BTEX' has not been included in this assessment.
- The EUSES model underestimated regional background concentrations of benzene in air in the United Kingdom although the predictions were generally within an order of magnitude of measured values. It was not possible to take account of emissions of benzene across Europe (other than from EPER sources) because a complete Europe wide emission inventory was not available.
- The EUSES model indicated that there are potential exceedences of the air quality limit value for benzene close to some EPER sources, based on conservative default assumptions concerning local dispersion. Maps prepared to present the EUSES model outputs clearly showed the location of these hot spots. Further EUSES modelling with more representative values for factors governing local dispersion (especially stack height) should be undertaken to determine if detailed local modelling or monitoring of benzene concentrations near to these sources is necessary.

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(77) It is interesting to compare these values to measurements reported in the EU draft risk assessment for benzene, made in the 1990s, which showed 'typical' concentrations of benzene in urban air in the range 10 to 20 μg m^{-3}.

4.2.5 *Arsenic assessment*

The EPER database listed 529 emissions of arsenic from 471 facilities. The emissions were to all three media: 227 to air, 232 direct to water and 70 indirect to water. Of the reported emissions, 319 were measured, 80 were estimated and 130 were calculated.

Major man-made sources of arsenic released to the environment are the metal industry, combustion processes and chemical manufacture. Drainage water from mines can be a significant source of arsenic pollution in the aquatic environment. Arsenic is a naturally occurring element present in rocks and soils.

Arsenic is harmful to humans and wildlife. The following Risk Phrases are relevant to exposure via the environment: R23/25 — 'Toxic via inhalation and if swallowed' and R50/53 — 'Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment' ([78]). Arsenic is not on any of the lists of Priority Chemicals under Council Regulation (EEC) 793/93. EUCLID and OECD Chemical datasheets are not available.

Official estimates of national emissions obtained from the EMEP Internet WebDab site were used to estimate regional and continental emissions to air and are shown in Table 28. Note the wide variation between countries in reported emissions, which is similar to the position regarding releases of hexachlorobenzene given in Table 21. We have not attempted to account for the wide country-to-country variation.

Table 29 shows the physical and chemical properties of arsenic used for the model runs. The Technical Guidance Document advises that water solubility, boiling point and vapour pressure data cannot be used for metals. It also advises that the use of the octanol-water partitioning coefficient is not appropriate and measured partition coefficients should be used instead for soil, sediments and suspended particulates. Empirical soil-water partitioning coefficient used for this assessment was taken from the US EPA Human Health Risk Assessment Protocol assuming a pH value of 7. It was assumed that the same partitioning coefficient applied to all solid media following the Human Health Risk Assessment Protocol.

Figure 16 shows the local predicted environmental concentration of arsenic in air, based on the EUSES modelling with default input parameters, which will result in highly conservative estimates. The highest predicted concentration was 1 220 ng m^{-3}. Predicted regional background concentrations were in the range 0.2–0.36 ng m^{-3}.

Parties to the Convention on Long-range Transboundary Air Pollution perform monitoring of arsenic at regional monitoring sites across Europe. Table 30 shows the measured arsenic concentrations at these sites during 2002. The measured concentrations at these sites are in the range 0.131–1.55 ng m^{-3}, which is comparable with the predicted regional background environmental concentrations of 0.2–0.36 ng m^{-3}.

Table 31 shows measured arsenic concentrations near industrial sites reported in the European Commission Position Paper on arsenic, cadmium and nickel ([79]). Table 32 shows more recent monitoring data (2002) from UK industrial sites ([80]). Generally these concentrations are substantially higher than those measured at regional background sites but considerably less than the local concentrations predicted by EUSES.

Table 28 Official estimates of arsenic emissions, 2002

Country	Emission, kg/year
Austria	Not available
Belgium	2 785
Germany	Not available
Denmark	767
Spain	60 487
Finland	3 741
France	24 460
Greece	0
Ireland	564
Italy	Not available
Luxembourg	Not available
Netherlands	912
Portugal	0
Sweden	809
United Kingdom	24 016
Total	

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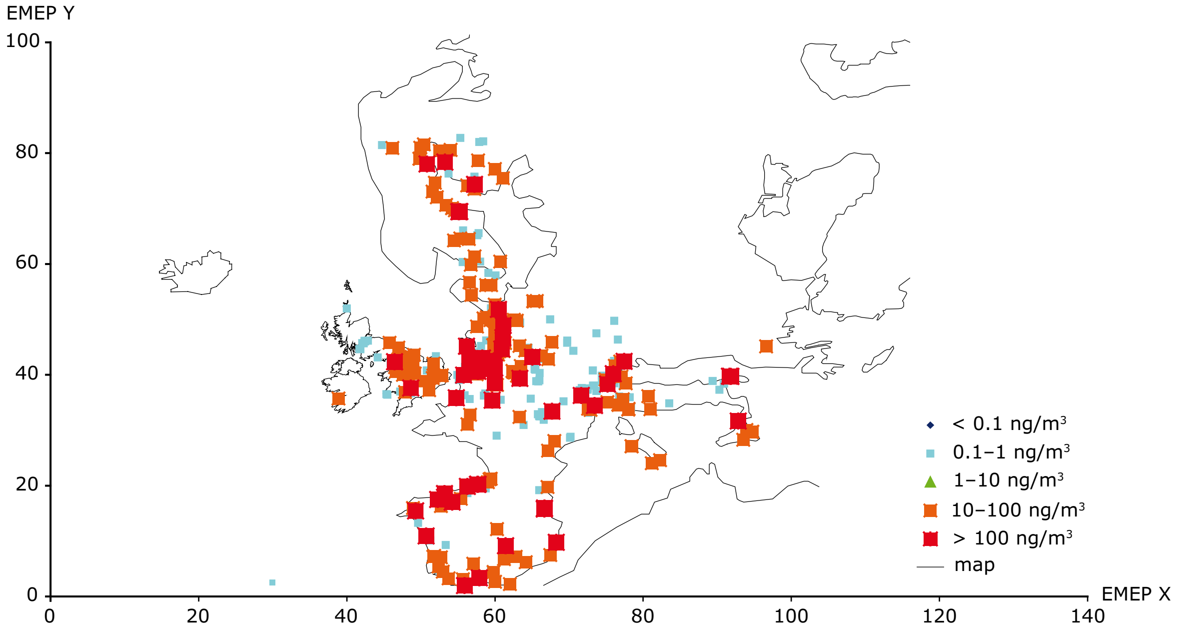
[78] http://ecb.jrc.it/esis/esis.php?PGM=ein.

[79] http://europa.eu.int/comm/environment/air/pdf/pp_as_cd_ni.pdf.

[80] http://www.airquality.co.uk/archive/data_and_statistics.php.

Figure 16 Predicted environmental concentrations of arsenic in air close to EPER sources of arsenic emissions



Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicate the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

Table 29 Properties of arsenic used in the assessment

Property	Value
Molecular weight	74.92
Melting point, °C	Not applicable
Boiling point, °C	Not applicable
Vapour pressure, Pa	10^{-20}
Temperature of vapour pressure measurement, °C	20
Log K_{ow}	Not applicable
Solubility (mg l^{-1})	10^{-20}
Temperature of solubility measurement, °C	25
Degradation rate in air, day^{-1}	0
Henry's law constant, Pa m^3 mol^{-1}	10^{-20}
Solids-water partition coefficient: soil, l kg^{-1}	29
Solids-water partition coefficient: sediment, l kg^{-1}	29
Solids-water partition coefficient: suspended matter, l kg^{-1}	29

The predicted concentrations in air may be compared with the 6 ng m^{-3} target value set in the Fourth Daughter Directive. Regional background concentrations predicted by EUSES are substantially less than the target value: however local concentrations predicted by EUSES are markedly greater than the target value (although measured concentrations may not be). The EUSES predictions of local concentrations are intended to be conservative and so the dispersion model predicts ground level concentrations at a distance of 100 m from the source assuming the whole of the emission is released through a 10 m high stack without buoyancy or momentum. More detailed assessment of local conditions is therefore required for these sources. The effect of better information on local dispersion on the local PEC for arsenic is demonstrated in the following example.

Table 30 Arsenic concentrations in air at background sites

Site	Measurement type	Concentration, ng m^{-3}
AT0002R	pm10	1.059
AT0005R	pm10	0.466
DE0001R	aerosol	0.613
DE0002R	aerosol	0.558
DE0003R	aerosol	0.202
DE0004R	aerosol	0.479
DE0005R	aerosol	0.427
DE0007R	aerosol	0.864
DE0008R	aerosol	0.433
DE0009R	aerosol	0.637
DK0003R	aerosol	0.676
DK0005R	aerosol	0.517
DK0008R	aerosol	0.333
DK0031R	aerosol	0.235
FI0036R	aerosol	0.186
GB0014R	aerosol	0.692
GB0090R	aerosol	1.55
GB0091R	aerosol	0.492
IS0091R	aerosol	0.131
LV0010R	aerosol	0.611
LV0016R	aerosol	0.855
NL0009R	aerosol	0.669
NO0042G	aerosol	0.39
NO0099R	pm10_pm25	0.062
NO0099R	pm25	0.236
SE0005R	aerosol	0.089
SE0014R	aerosol	0.389
SK0002R	aerosol	0.242
SK0004R	aerosol	1.033
SK0005R	aerosol	1.3
SK0006R	aerosol	0.693
SK0007R	aerosol	1.679

Table 31 Arsenic concentrations measured near industrial sites (European Commission Position Paper on arsenic, cadmium and nickel)

Location, environment	Sampling period	Concentration ng m^{-3}	Notes
Industrial			
Hamburg, Germany	1997/1998	5 and 13	Secondary copper smelter, distance 1 000 m, windward, lee
Datteln, Germany	1997	9	
Datteln, Germany	1998	14.3	Vicinity of zinc smelter
Stolberg, Germany	1997	4	Vicinity of zinc smelter
Stolberg, Germany	1998	2.3	Lead smelter
Kokkola, Finland	1993	1.7	Distance 600 m
Kokkola, Finland	1993	1.2	Zinc industry, distance 1 500 m
Raahe, Finland	1998	1.2	
Harjavalta, Finland	1995	27	Zinc industry distance 4 000 m
Harjavalta, Finland	1996	24	
Harjavalta, Finland	1997	20	Near iron and steel plant
Harjavalta, Finland	1995	21	Copper/nickel smelter
Harjavalta, Finland	1996	16	Distance 1 000 m
Harjavalta, Finland	1997	16	
Hoboken, B	1998	97	Lead-copper smelter, range of several sampling points, distance up to 250 m
Duisberg, Germany	1998	11	
Duisberg-Bruckhausen, Germany	1999	4	Lead copper smelter (industrial hot spots) 150 m from non-ferrous industry, half yearly average
Beverwijk, Netherlands	1998/1999	0.9	
Hock van Holland, Netherlands	1998/1999	0.98	700 m windward of steel mill, 1/1999–10/1999 near steel mill petrochemical industry

Table 32 Arsenic concentrations measured in air near industrial sites in the United Kingdom, 2002

Site	Concentration, ng m^{-3}
IMI (2) Refiners, Walsall	1.92
Corus Steel, Rotherham	2.70
Cerro Extruded Metals, West Bromwich	1.71
Walkers Galvanizing, Wallsall	1.63
White Rose Environmental, Leeds	1.65
Bruhl UK Ltd, Sandwell	2.53
Sidney Smith, Ambelcote, Stourbridge	1.99
BZL, Hallen	4.79
Avesta Polarit, Rotherham	2.37
Brookside, Bilston Lane	1.82
Elswick (6), Newcastle	1.74

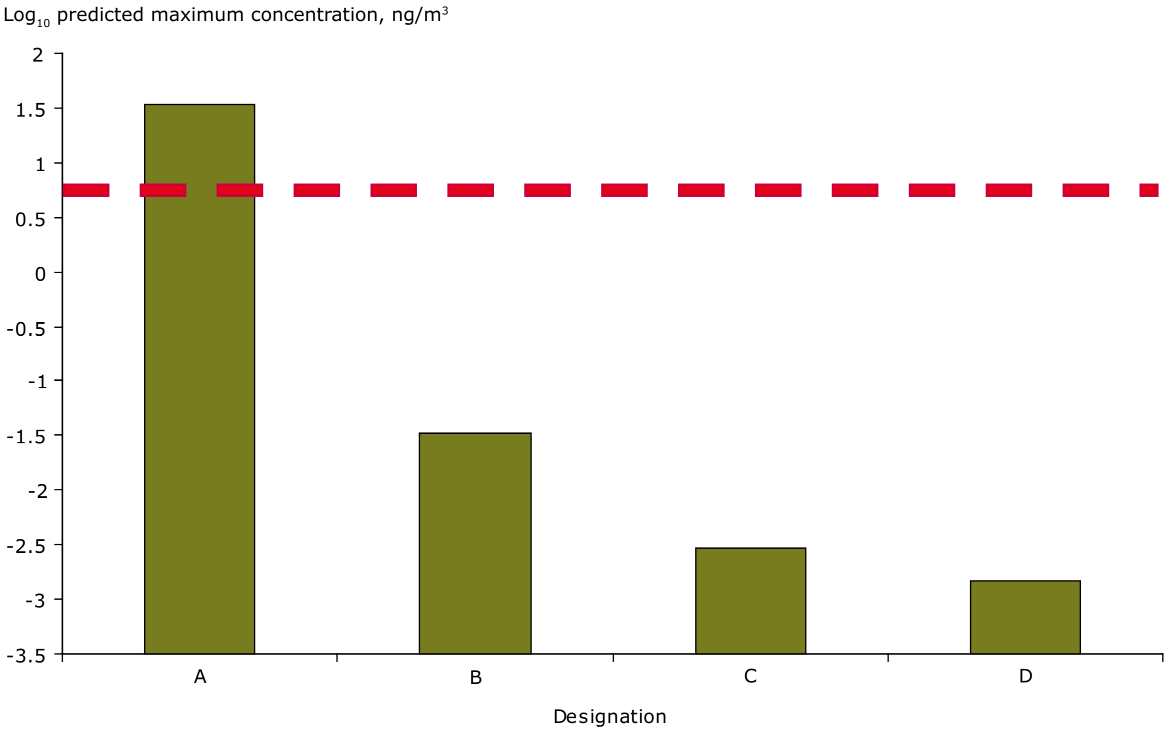
Box 6 considers a large coal-burning power station in the United Kingdom: it shows how the estimates of pollutant concentrations change as more local details are taken into account. The resulting maximum predicted concentrations obtained, as successively more information is available is plotted as a graph in Figure 17. Note the logarithmic scale and the comparison with the fourth daughter directive target represented by the dashed horizontal line. By taking account of the actual height of the stack (in 'B'), it can be seen that the predicted local concentration falls well below the target value. Further reductions in PEC result when additional information on plume characteristics and local dispersion are successively included in the model input, as shown by cases C and D in Box 6 and Figure 17.

Figure 18 shows predicted environmental concentrations of arsenic in surface waters close to EPER sources. The maximum predicted concentration was 447 µg/l. Background concentrations in rivers in the United Kingdom were in the range 0.5–2.2 µg/l in 2003 (81).

Member States were required to establish pollution reduction programmes for arsenic including water quality objectives according to Article 7 of Council Directive 76/464/EEC. The United Kingdom set a quality standard of 50 µg/l for inland waters. The EUSES modelling predicted that concentrations of arsenic in surface waters would exceed this standard at several locations throughout Europe close to EPER sources. However, the EUSES model is intended to provide a conservative estimate of pollutant concentrations. Further screening with EUSES, based on sector or region specific information on dilution rates, type of wastewater treatment plants etc. would be needed to determine the requirement for more detailed local modelling or monitoring close to the sources identified.

Figure 19 shows predicted environmental concentrations of arsenic in agricultural soils close to EPER sources. The maximum predicted concentration was 1.73 mg/kg wet weight of soil. However, it should be noted that arsenic occurs naturally in rocks and soils. Uncontaminated soils generally contain approximately 10 mg/kg (82).

Figure 17 Effects of increasing data availability on predicted concentrations of arsenic in air



Note: Log plot of predicted maximum concentration of arsenic in air with increasing information on the discharge and dispersion characteristics. The graph is based on the data shown in Box 6. The dashed horizontal line corresponds with the 6 ng/m^3 limit specified under the Fourth Daughter Directive.

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(81) http://www.defra.gov.uk/environment/statistics/inlwater/iwhmetal.htm#iwtb11.

(82) B.J Alloway: Heavy metals in soils, Halsted Press 1990.

There are no general EU limits for arsenic content of soil. In the United Kingdom a Soil Guideline Value for arsenic in allotment areas used for growing vegetables of 20 mg/kg dry weight has been set (83): for industrial areas the Soil Guideline value is 500 mg/kg dry weight. Allowing for a soil solids content of 60 % by volume, a soil water content of 20 % by volume and a soil bulk density of 1 700 kg m^{-3} the soil guideline values are equivalent to approximately 17.6 mg/kg and 440 mg/kg on a wet weight basis.

Comparing the predicted concentrations with the Soil Guideline Values, it is concluded that EPER sources are unlikely to lead to exceedance of the soil guideline value except where background soil concentrations are already high.

Box 6 Case study of the effect of taking account of local conditions on predicted pollutant concentrations

The EPER database provides an emission estimate of annual emissions to air of 45 kg of arsenic from a large UK coal-fired power station. The EUSES model, without any additional information about local conditions (EUSES default), predicts a local concentration of 34.3 ng m^{-3}, well in excess of the 6 ng m^{-3} target value set in the Fourth Daughter Directive. The results of increasingly more detailed modelling shown below demonstrate that the emission from this source will not lead to exceedence of the target value.

Designation used in Figure 17	Additional local information	Model	Maximum concentration in air at source strength of 1 kg per day, mg m^{-3}	Maximum predicted concentration, ng m^{-3}
A	None	EUSES default	2.78×10^{-4}	34.3
B	Stack height = 198 m	EUSES. Environment Agency Horizontal Guidance Note H1. (84) The Guidance Note presents a table of maximum ground level concentrations for various stack heights based on modelling using ADMS3 for worst case meteorological conditions assuming no plume rise	2.66×10^{-7}	0.033
C	Stack height = 198 m Effective stack diameter = 12 m Discharge temperature = 130 °C Discharge velocity = 27 m s^{-1}	EUSES. Environment Agency Guidance for estimating the air quality impact of stationary sources. The guidance provides a series of nomographs based on ADMS for various stack heights for typical UK meteorological conditions taking account of plume buoyancy and momentum	2×10^{-8}	0.003
D	As above Hourly sequential meteorological data for region Time varying emissions profile for UK coal-fired power stations	ADMS 3.2	1.2×10^{-8}	0.0015

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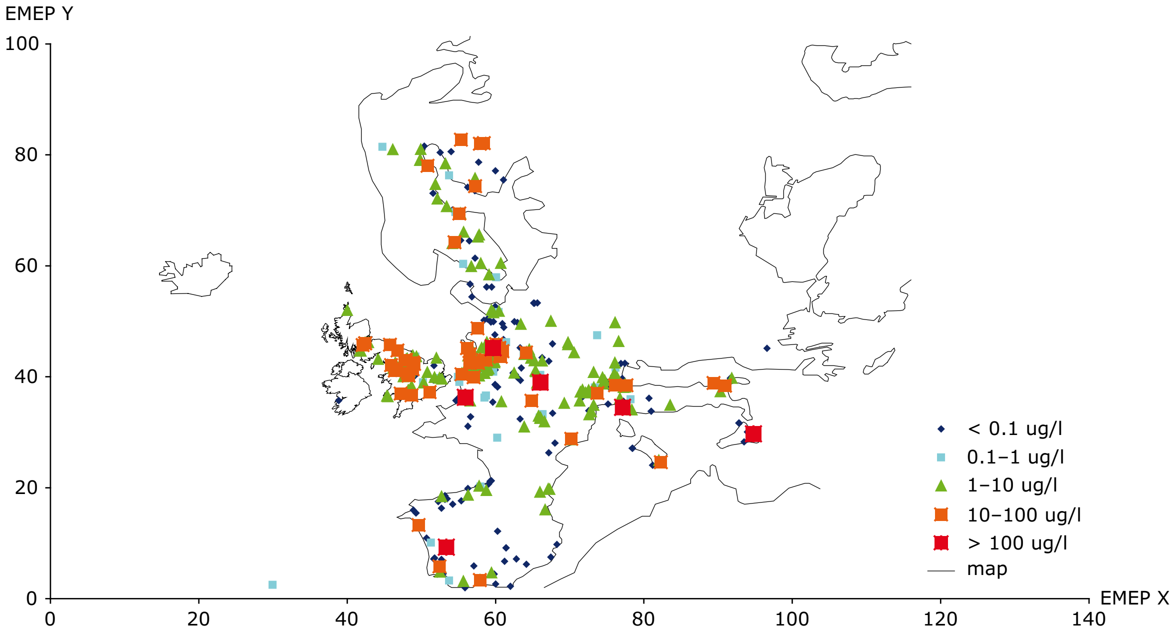
(83) http://www.environment-agency.gov.uk/commondata/acrobat/sgv1_arsenic_676042.pdf

(84) Environment Agency. Integrated Pollution Prevention and Control (IPPC) Environmental Assessment and Appraisal of BAT. Horizontal guidance Note H1. http://www.environment-agency.gov.uk/commondata/acrobat/h1v6_jul03guidance_608809.pdf

The following **conclusions** may be drawn from the assessment for arsenic:

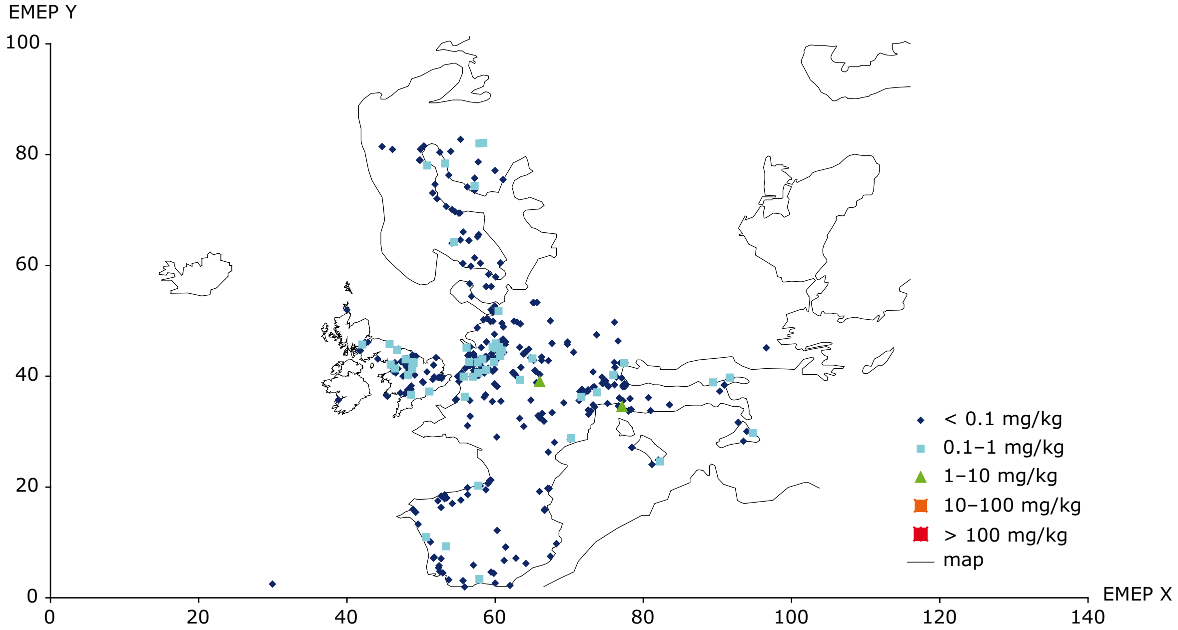
- The EPER database lists a large number of emission sources to air and water.
- National estimates of arsenic emissions to air are available from the EMEP WebDab for many countries.
- EUSES predictions of arsenic concentrations in air are comparable with measured concentrations at background locations throughout Europe.
- Measured and modelled regional background concentrations in air are substantially less than the target value set in the Fourth Daughter Directive.
- The EUSES model indicated that there are potential exceedances of target values for arsenic in air close to some EPER sources, based on conservative default assumptions concerning local dispersion. Maps prepared to present the EUSES model outputs clearly showed the location of these hot spots. Further EUSES modelling with more representative values for factors governing local dispersion (especially stack height) should be undertaken to determine if detailed local modelling or monitoring of arsenic concentrations near to these sources is necessary.
- The effect of taking more realistic input data relating to stack height, plume characteristics and local dispersion to substitute for the default parameters values in EUSES in terms of markedly reducing local PEC of arsenic in

Figure 18 **Predicted environmental concentrations of arsenic in surface waters close to EPER sources of arsenic emissions**



Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicate the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

Figure 19 Predicted environmental concentrations of arsenic in agricultural soils close to EPER sources of arsenic emissions (wet weight basis). PEC excludes contribution from soil minerals



Note: The map shows the predicted environmental concentrations for facilities located at the positions given in the EPER database, calculated using the default parameter values (i.e. not based on specific information relating to each facility) for the EUSES model. The size, shape and colour of the markers indicate the concentrations calculated for emissions at the locations shown. For local concentrations, these refer to concentrations within 100 metres of the emission. Regional concentrations due to each source are averaged over a 200 x 200 km area centred on each emitting facility. Because of the sensitivity of local concentrations regarding the degree of dilution and dispersion of substances immediately following their release, the results shown for such cases must be regarded as illustrations only. In most cases, predicted environmental concentrations in the locality of an emission (especially to air) will be substantially lower when based on site-specific, as opposed to default, parameter values in EUSES. See text for details.

air has been demonstrated with the example of emissions to air from a coal-fired power station.

- Local concentrations in surface waters predicted by EUSES in the vicinity of several EPER sources exceed national standards set by some countries in response to Council Directive 76/464/EEC. Further screening with EUSES with region or sector specific information on factors such as dilution rates and type of wastewater treatment plants should be used to determine the need for detailed modelling or monitoring of arsenic close to these sources.

- The EUSES model predictions of the concentrations of arsenic in agricultural soils have been underestimated because the natural content of the soils has not been taken into account.

- The EUSES model predicts that the concentrations of arsenic in soils close to EPER sources are not likely to exceed the soil guideline value except where the inherent content of the soil is high.

4.2.6 Demonstration of how screening model outputs may be overwritten with more accurate information

The strategy proposed in Section 4.1 envisaged that when better data is located for modelled regional or local predicted environmental concentrations, then this data may be substituted for the screening model predictions. This approach was illustrated in the flow chart in Figure 8. It is easiest to demonstrate the application of the flowchart by means of example.

For arsenic, the initial EUSES screening indicated that the air and water quality standards might be exceeded on the local scale close to the emission source, but not more generally on the regional scale. The next stage in this case would be to undertake further modelling with EUSES using sector-specific estimates for parameters affecting local dispersion, particularly stack height, to reduce the inherent high level conservatism of the output based on the default input assumptions. Box 6 and Figure 17 demonstrated the potential benefits of taking account of local detailed information in relation to emissions to air. If the EUSES modelling with sector specific input data also indicated possible exceedance of relevant standards on the local scale, then this would signal the need for detailed modelling or other investigation.

The results of more detailed modelling can be used to overwrite default values within EUSES. We envisage that individual companies could provide optional additional information to the national regulator responsible for the collation of EPER data. The information might include:

- the EUSES parameter identifier;
- the parameter value, in appropriate units;
- a data source reference, for quality assurance purposes.

The additional information would be used by EUSES to provide better estimates of the impact from each source. The national regulator would then be responsible checking that the additional information provided is valid.

Consider the case study shown in Box 6. The operator may wish to include information on the air dispersion factor (the maximum concentration in air at unit source strength) based on detailed dispersion modelling. The data return for the arsenic emission from the power station would then include:

- the EUSES parameter identifier, PA CstdAir;
- the parameter value, 1.2×10^{-14} (kg m^{-3})/(kg d^{-1});
- a reference to the dispersion modelling study.

4.2.7 *Assessment of the usefulness of the EPER data format*

The assessments carried out for hexachlorobenzene, benzene and arsenic have demonstrated that the EPER data can be readily used together with the EUSES risk assessment model to provide useful screening assessments of the potential impact of the emissions on concentrations in the environment.

The format of the EPER database allows the data to be extracted readily to provide the input to chemical fate models by means of simple computer scripts. The database gives details of the geographical location of each source and so it is relatively straightforward to prepare maps of pollutant hot spots associated with EPER sources. The provision of the details of the geographical location of the site also greatly facilitates the extraction of site-specific environmental data for modelling from climate, land cover and river catchment databases.

To some extent, the EPER database duplicates the information already held in the EMEP large point source inventory. However, the EPER database has the following benefits:

- it provides information on emissions to both air and water;
- it can contain information on pollutants other than those covered by the Convention on Long-range Transboundary Air Pollution;
- the EMEP large point source inventory is only prepared once every five years whereas the EPER database will eventually be updated more frequently;
- the EMEP large point source inventory only covers large sources: the EPER database includes smaller plant because reporting thresholds are lower.

The EMEP large point source database provides information on the height of discharge above ground: this element is not available from the EPER database. It would be useful for the calculation of local and regional air concentrations, which are dependent on the height of emission.

We have considered whether the EPER data provides added value for both high and low resolution assessments. Our experience with hexachlorobenzene, benzene and arsenic modelling suggests that the EPER database does not contain sufficient information to allow a high-resolution detailed assessment to be carried out. For example, a detailed local assessment of air dispersion would require additional information about discharge stack heights and diameters, the temperature and velocity of discharge and local topographical details. The format of the data is however ideally suited to low resolution-screening assessments of large numbers of sources.

The EPER data may increase the usefulness of existing models on the (pan) European and regional level because it contains data for many more point sources than the existing data sources. Currently, it is often necessary to spatially disaggregate national or regional emission totals onto an emissions grid for modelling purposes. The EPER data will allow more precise allocation of emissions onto the model grid.

A further limitation on the usefulness of the EPER data relates to the level of detail available for individual chemical substances. Several chemicals of interest exist in a large number of closely related forms (isomers or congeners), for example, polycyclic aromatic hydrocarbons, (PAHs), 'dioxins and furans', polychlorinated biphenyls and polybrominated diphenyl ethers. Individual chemical species within these families of compounds often have markedly different environmental and biological properties, yet the database reports these complex mixtures as though they are single compounds. Similar difficulties arise with other chemicals that are reported as mixtures — for example, 'BTEX', which is an undefined mixture of benzene, toluene, ethylbenzene and the three isomers of xylenes. In these cases, modelling will depend on the availability of additional information on typical emission compositions relevant for the processes of interest, but this will introduce a further source of uncertainty.

4.2.8 Specifying the requirements for more detailed modelling

The output from the EUSES model may be used to specify the requirements for more detailed modelling. The basic approach is to compare the predicted contribution from the EPER sources with environmental quality criteria and background concentrations at the local, regional, continental and possibly global scales. More detailed modelling is required where EUSES indicates that the EPER sources have the potential to have adverse affects on human health or the environment. The two main considerations for the selection of more detailed assessment are:

- the scale of the potential impact-local, regional, continental or global;

- the media affected-air, water, soil or multi-media and whether the pollutant is transferred between media from emission to potential impact.

If the critical potential impact occurs in the same medium as the pollutant was emitted, then the more detailed model should treat the transfer of the pollutant through that medium in greatest detail. Many of the models identified in Part 1 of this report are concerned with pollutant transfer through a single environmental medium. However, if the critical impact is predicted to occur in a different medium then a multi-media model is required. In many cases, it will be appropriate to combine spatially resolved air or water dispersion model with a local multi-media model. For example, it is often effective to use a local air dispersion model to predict ground level concentrations and rates of deposition at relevant receptor locations and then use a simple multimedia model to predict the distribution of the pollutant into other media at each receptor location. This approach is widely used to assess the impacts of emissions of dioxins and PCBs from waste incinerators on the food chain.

Consideration of the scale of the potential impacts identified by EUSES leads directly to the choice of the model scale. Local scale impacts demand local-scale models: global scale impacts demand global scale models. Table 33 provides indicative dimensions of the respective model domains and model resolution.

This feasibility study has indicated that the critical impacts associated with EPER emissions are often local to the source of the emission. The ability to model local impacts in detail requires more information on the discharge than are currently provided in the EPER database. The required information is not always readily available. We have therefore attempted to rank the required information in terms of its importance for modelling of releases to air and directly or indirectly to water. Table 34 shows how we have ranked the information required in four tiers:

- Tier 1: The existing information in the EPER database
- Tier 2: The minimum additional information required for modelling purposes
- Tier 3: Further easily specified information
- Tier 4: Other details that may influence pollutant impacts, but are not readily specified in general terms.

We have assumed that information on the local environment — its meteorology, topology, land cover etc., is available from other sources.

In general, it will be useful to reassess the potential impact of the EPER sources at the local level with the new data using simple screening tools such as EUSES prior to more detailed modelling. Table 34 showed how screening models can be used to reassess potential impacts as more information becomes available.

4.3 Work plan for predicting chemical density from EPER releases

This section provides an outline work plan on how the staged approach to predicting chemical density demonstrated in the previous section may be extended to all appropriate EPER substances. It corresponds with the work defined under Task 7 of the technical specification (Appendix 1) of this feasibility study. It also builds on the discussion of the modelling strategy (presented in Section 4.1) that took place at the expert workshop in Copenhagen on 16 August 2005, at which a draft of this final report was reviewed. The summary proceedings of this workshop are given in Appendix 4.

Delegates at the expert workshop were in overall agreement that the staged approach to modelling set out in Section 4.1.2, based on EUSES for screening to identify circumstances where more detailed modelling is required, is appropriate. For the impact of emissions on concentrations in the environment *local* to the emission source, information on the local dispersion following release has a major impact on the predicted local concentrations. This information (which includes details of stack height, plume buoyancy, dilution rates into water, type of wastewater treatment plant etc.) is either not in the public domain or else very difficult to access. The use of default values for these parameters in EUSES results in very conservative predictions (at least

Table 33 Indicative model domains and resolution

Scale	Indicative dimension of model domain	Indicative model resolution
Local	Up to 50 km	Stack height for air dispersion modelling Water depth for detailed hydrodynamic modelling
Regional	200 km	2 km
Continental	EMEP grid	10–150 km
Global	Global	2°

Table 34 Model input information hierarchy

	Emission route		
	Air	**Direct to water**	**Indirect to water**
Tier 1 (EPER)	Emission Location	Emission Location	Emission Location
Tier 2	Stack height	Nature of receiving waters-river, coastal etc. Dilution factor	Effluent discharge rate of STP Type of treatment plant — e.g. trickling filter, activated sludge, anaerobic digestion etc. ←
Tier 3	Stack diameter Volume flow rate Discharge temperature Local surface roughness	Sediment concentrations Temperature of emission Temperature of receiving waters Local solid-water partition coefficients	SimpleTreat input parameters(see Table 35, below) ←
Tier 4	Temporal emissions and discharge rate profiles Details of buildings affecting dispersion Details of local terrain Details of local exposure	Local river/tidal flow patterns and turbulence patterns Temporal and spatial emissions and discharge rate profiles	

Table 35 Simple treat input parameters

Temperature of air above aeration tank
Temperature of water in aeration tank
Depth of primary settler
Hydraulic retention time of primary settler
Density of suspended and settled solids in primary settler
Fraction of organic carbon in settled sewage sludge
Depth of aeration tank
Density solids of activated sludge
Activated sludge solids concentration
Steady state oxygen concentration in activated sludge
Mode of aeration
Rate of aeration for diffuse aeration
Fraction of organic carbon in activated sewage sludge
Sludge loading rate
Hydraulic retention time in aerator
Sludge retention time of aeration tank
Depth of solids-liquid separator
Density of suspended and settled solids in solids-liquid separator
Concentration of solids in the effluent
Hydraulic retention time of solids-liquid separator
Fraction of organic carbon in effluents sewage sludge

for releases to air). Delegates agreed that it is not possible to accurately model local environmental concentrations resulting from EPER emissions sources using publicly available input data only: detailed release and local dispersion information would be required too, and obtaining this site-specific information would be problematical.

The strategy (in Section 4.1) proposed an approach by which operators could be prompted to provide local concentration data on a voluntary basis through consultation and the publication of local screening predictions on a website. This would encourage industry to provide better information on local concentrations to overwrite the more conservative screening model estimates. The strategy recognised that some of this information may be held on the public record (for example, in IPPC permit applications), and so seeking information via this route could provide an additional source of information on local concentrations to replace screening model predictions. However, delegates agreed that publication of modelled predictions of local concentrations could be highly contentious with industry and local regulators. Further consideration of whether and how to provide public information on local concentrations of chemicals resulting from point source emissions requires further detailed consideration that is outside the scope of this modelling feasibility study. Publication of the results of any modelling of local environmental concentrations should there not take place until this issue is resolved. Regarding the acquisition of information on local concentrations from information on the public record, for example, IPPC permit applications, delegates agreed that this was likely to be highly problematical. Pilot studies could be undertaken to provide a more detailed assessment, based on selected regions where the national and local authorities are prepared to share information.

With the exception of that part of the part of the strategy concerned with obtaining information on local concentrations where accurate modelling cannot be undertaken due to lack of detailed site-specific data, delegates endorsed the approach and strategy proposed in the draft final report, as described in Section 4.1.2 of this document. The work plan presented below reflects these workshop conclusions.

4.3.1 Proposed work plan

A two-phased approach to the work plan is proposed: the first phase would involve two stages of screening with EUSES, the outcome of which would inform the need for detailed modelling with spatially resolved models, if necessary, in the second phase. The approach is summarised below and the various tasks are described in further detail.

The first phase would require the EUSES model to be run using default release and landscape input data for relevant substances listed in EPER, as undertaken for the test substances in the previous section. The predicted environmental concentrations would then be compared with relevant standards or monitoring data and emissions predicted to cause exceedances of the relevant criteria would then be identified. The modelling would focus on regional (and greater) spatial scales.

EUSES would then be re-run, focussing on substances showing exceedances in the first screening run, using location and sector specific information, such as release data, river flow data, and geographical and meteorological data representative of the region of the release. This part of the study would include uncertainty analysis and identification of output sensitivities to key input variables. The resulting predicted environmental concentrations on the regional and greater scale would then be compared again with the relevant criteria, identifying any cases of exceedances. Chemicals showing exceedances would then be candidates for detailed modelling in the second phase of the study.

Following completion of this analysis, the results would be summarised in the Phase 1 interim report, which would be presented at an expert workshop. The workshop delegates would provide feedback on the work so far and the proposed approach for detailed modelling in Phase 2. A costed proposal for the Phase 2 work then be included as part of the Phase 1 final report.

The second phase of the study cannot be defined in detail now as this will be determined by the results obtained in the first part of the proposed work plan. However, it is envisaged that this will entail detailed modelling of a limited number of substances of concern selected as a result of the Phase 1 work. It is proposed that a further expert workshop would be convened to peer-review the output. The results of regional plus scale modelling should be made publicly available on a website, in accordance with the principles of public access to environmental data.

Further details of the proposed work plan and the indicative costs for Phase 1 are given below.

We envisage the first phase of the study to involve the following tasks:

- **Task A** (85) **— Initial EUSES modelling.** Prepare a prioritised list of chemical releases from EPER sources, develop assessment criteria, identify relevant model outputs and run the EUSES model with default parameter values, identifying potential exceedences of environmental quality criteria on local and regional scale.
- **Task B — Further EUSES modelling.** Re-run EUSES for releases showing exceedences with sector- and location-specific input data, explore key sensitivities and uncertainties. Identify candidate substances for detailed modelling in Phase 2.
- **Task C — Phase 1 interim report.** Prepare a detailed report of the work so far, including conclusions and recommendations for detailed modelling in Phase 2.
- **Task D — Expert workshop.** Review the progress so far and agree the strategy for Phase 2.
- **Task E — Phase 1 Final report.** Revise the interim report in the light of the workshop discussions and prepare detailed work plan and costs for extending the work into Phase 2.

Task A — Initial EUSES modelling
We envisage that work under Task A would address the following topics:

- selection of a list of candidate chemicals for modelling and definition of required outputs;
- identification of sources of monitoring data;
- identification of relevant environmental quality criteria;
- preparation of scripts for running EUSES;
- modelling and results evaluation.

As outlined above, Task A would involve running the EUSES model for a prioritised set of chemicals reported under EPER, using the default EUSES model parameters. We propose that the chemicals would be grouped according to their principal environmental effects and concerns, availability of

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(85) Tasks in the proposed workplan are number alphabetically to avoid confusing with tasks in the present study.

monitoring data and broad types of emission source. This categorisation is shown on a pragmatic basis in Table 36. In addition to the substances listed in EPER, the table also includes additional substances that will be reported under the proposed European Pollutant Release and Transfer Register (EPRTR) (86) due to come on line in 2007. Consideration of the environmental properties of the chemicals of interest will also help to determine the media and geographical scale of EUSES modelling that will be of greatest relevance, as illustrated in Table 20 in Section 4.2.2.

Several of the chemicals listed in Table 36 with particular types of impact may be excluded from further analysis: chemicals for which the only significant impacts are global warning or stratospheric ozone destruction will not require further analysis as these impacts do not require localisation to particular sources. Regional acidification and eutrophication effects resulting from emissions of oxides of sulphur and nitrogen, and ammonia, into the atmosphere is the subject of intensive modelling studies to determine deposition rates and critical load exceedances that further specific modelling of emissions is unnecessary. Similarly, the production of ground-level ozone and other photochemical oxidants from VOCs and NO_X is already the subject of intense international modelling and hence it is not appropriate to duplicate this work. The outcome of this work is available from EMEP (87).

Table 36 also gives an assessment of the expected availability of monitoring data that would be required for comparison with model results. Regulation and legislative requirements are the main drivers for environmental monitoring: consequently substances that are already the subjects of regulation are the ones for which most monitoring data are available. The availability of monitoring data for air, surface water and sediments, soils and biota is indicated on a simple three-point scale in the table, based on the level of regulation of the substance in question. The table also contains a categorisation of the main types of source of emission, identifying point sources (i.e. releases from major industrial installation included in EPER) and diffuse sources (such as pesticide application and run-off, emissions from vehicle, domestic premises and minor industrial facilities not included in EPER). It also identifies chemicals where there is a significant natural source, in addition to man-made sources. Examples of chemicals having natural emissions are ammonia, dinitrogen oxide (nitrous oxide) and methane emissions to air, and heavy metals, chlorides and fluorides leaching into water from natural rocks and soils. We recommend that the study focus on chemicals where significant releases from EPER point sources are the main route of release to the environment. We note that many of the chemicals to be included in the EPRTR are POPs which have been phased out of use in Europe for many years (such as PCBs, 'drin' pesticides that have no history of usage in Europe). From previous analysis of emissions of these compounds reported on the United Kingdom's Pollution Inventory, we would anticipate that releases reported for these substances would be very low. In addition, a number of EPRTR substances are pesticides that have a more recent history of usage, such as alachlor, atrazine, chlorpyrifos etc., where the main release route will occur following application to crops and subsequent run-off or volatilisation, rather than from point sources of emissions.

A further issue for investigation concerns mixtures of closely-related chemicals that are currently reported in EPER or EPRTR as single substances. Examples of this include dioxins (88), PAHs and PCBs, where each single EPER entry in fact represents tens or hundreds of individual congeners, which vary in terms of chemical properties, harmfulness and environmental behaviour. To reduce the work to manageable proportions, the study should focus on the most significant congeners, based on international toxicity ranking. For the initial EUSES model runs, a worst-case analysis could be undertaken, in which EUSES is run repeatedly for the key congeners, assuming that the release consists only of the congeners of interest. Scripts to run EUSES would allow this to be undertaken reasonably quickly. The outputs would then be compared on the basis of toxic equivalency by multiplying the predicted concentrations of each congener by its Toxic Equivalent Factor. Should any of the results show an exceedance of the relevant criteria, then further modelling would be needed, using more detailed input data.

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(86) Proposal for a Regulation of the European Parliament and of the Council concerning the establishment of a European Pollutant Release and Transfer Register and amending Council Directives 91/689/EEC and 96/61/EC. COM(2004)634 final. 2004/0231 (COD) Brussels, 7.10.2004.

(87) http://www.emep.int/index_pollutants.html

(88) 'Dioxin' is the shorthand term for the family of polychlorinated dibenzo-p-dioxins and the related furans, about 200 substances in total, of which 17 are of toxicological significance. The toxicity of each congener is expressed in terms of toxic equivalent factors (TEF), which related the toxicity of individual congeners to the most toxic member of the group, 2,3,7,8-tetrachlorodibenzo-p-dioxin. The toxicity of a mixture of congeners (expressed as Toxic Equivalents, or TEQs) can then be determined as the sum of each congener multiplied by its own TEF.

Table 36 Possible groupings of EPER and EPRTR substances

			Monitoring data				Impacts and concerns											
Substance	**EPRTR substance**	**Sources**	Air	Water and sediment	Soil	Biota	Acidification	Eutrophication	O_3 formation	O_3 depletion	Local air pollution	Global warming	Heavy metals	Org water pollutant	POP or POP-like	Pesticide	Possible EDS	Inorg water pollution
See note No:	1	2	3	3	3	3	4	4	4	4	4	4	4	4	4	4	4/5	4
1,1,2,2-tetrachloroethane	X	D	3	3	3	3										X		
Alachlor	X	D	3	3	3	3										X		
Aldrin	X	D	3	3	3	3									X	(X)		
Ammonia, NH_3		P/D/N	1				X	X										
Anthracene	X	P/D/N	3	3							X							
Arsenic and its compounds		P/D/N	2	2	2	2					X		X					X
Asbestos	X	D	2								X							
Atrazine	X	D	3	1	2	3								X		X		
Benzene		P/D/N	1	1					X		X							
Benzene, toluene, ethylbenzene, xylenes (as BTEX)		P/D	1	1					X		X			X				
Brominated diphenylethers		D	3	3	3	3								X	X		X	
Cadmium and its compounds		P/D/N	2	2	2	2					X		X					X
Carbon dioxide, CO_2		P/D/N	1									X						
Carbon monoxide, CO		P/D/N	1								X							
Chlordane	X	D	3	3	3	3									X	(X)	X	
Chlordecone	X	D	3	3	3	3									X	(X)	X	
Chlorfenvinphos	X	D	3	2	2	3								X		X	X	
Chlorides		P/D/N		2	2													X
Chlorine and inorganic compounds (as HCl)		P/D/N	2				X				X							
Chloro-alkanes (C10-13)		D	3	3	3	3								X	X		X	
Chlorofluorocarbons	X	D	3							X		X						
Chlorpyrifos	X	D	3	2	2	3								X		X		
Chromium and its compounds		P/D/N	2	2	2	2					X		X					X
Copper and its compounds		P/D/N	2	2	2	2					X		X					X
Cyanides, total CN		P/D	3	3	3	3												X
DDT	X	D	3	3	3	3									X	(X)	X	
Di-(2-ethyl hexyl) phthalate (DEHP)	X	D	3	3	3	3					X			X	X			
Dichloroethane-1,2 (DCE)		P/D	3	3	3	3			X					X				
Dichloromethane (DCM)		P/D	3	3	3	3			X					X				

Table 36 Possible groupings of EPER and EPRTR substances — contd

			Monitoring data				Impacts and concerns											
Substance	**EPRTR substance**	**Sources**	Air	Water and sediment	Soil	Biota	Acidification	Eutrophication	O_3 formation	O_3 depletion	Local air pollution	Global warming	Heavy metals	Org water pollutant	POP or POP-like	Pesticide	Possible EDS	Inorg water pollution
See note No:	1	2	3	3	3	3	4	4	4	4	4	4	4	4	4	4	4/5	4
Dieldrin	X	D	3	3	3	3									X	(X)		
Dinitrogenoxide (N_2O)		P/D/N	3						X			X						
Dioxins and furans (PCDDs and PCDFs)		P/D/N	3	3	2	2					X				X		X	
Diuron	X	D	3	3	3	3								X	X	X		
Endosulphan	X	D	3	3	3	3								X	X	X		
Endrin	X	D	3	3	3	3									X	(X)		
Ethyl benzene	X	P/D		2					X		X			X				
Ethylene oxide	X	P	3								X							
Fluoranthene	X	P/D	2	2							X				X			
Fluorides		P/D/N		2	2	2												X
Fluorine and inorganic compounds (as hydrogen fluoride)		P	2								X							
Halogenated Organic Compounds (AOX)		P		1										X				X
Halons	X	D	3							X								
Hexabromobiphenyl	X	D	3	3	3	3									X			
Hexachlorobenzene (HCB)		D	3	3	3	3					X				X	(X)	X	
Hexachlorobutadiene (HCBD)		D	1						X		X							
Hexachlorocyclohexane (HCH)		D	3	3	3	3								X	X	X	X	
Hexachlorofluorocarbons (HCFCs)	X	D	3							X		X						
Hydrofluorocarbons (HFCs)		D	3									X						
Hydrogen cyanide (HCN)		D	3								X							
Isodrin	X	D	3	3	3	3									X	(X)		
Isoproturon	X	D	3	3	3	3								X		X		
Lead and its compounds		P/D/N	2	2	2	2					X		X					X
Lindane	X	D	3	2	2	2								X	X	X		
Mercury and its compounds		P/D/N	2	2	2	2						X	X		X	(X)		X
Methane, CH_4		P/D/N	2									X						
Mirex	X	D	3	3	3	3									X	(X)	X	
Naphthalene	X	P/D/N	3	3	3	3								X				
Nickel and its compounds		P/D/N	3	3	3	3					X		X					X

Table 36 Possible groupings of EPER and EPRTR substances — contd

Substance	EPRTR substance	Sources	Monitoring data				Impacts and concerns											
			Air	Water and sediment	Soil	Biota	Acidification	Eutrophication	O_3 formation	O_3 depletion	Local air pollution	Global warming	Heavy metals	Org water pollutant	POP or POP-like	Pesticide	Possible EDS	Inorg water pollution
See note No:	1	2	3	3	3	3	4	4	4	4	4	4	4	4	4	4	4/5	4
Nitrogen oxides, NO_x		P/D	1				X	X	X		X							
Nitrogen, total		P/D/N		1				X										X
Non methane volatile organic compounds (NMVOC)		P/D/N	1						X		X							
Nonylphenol ethoxylates (NP/NPEs)	X	P/D		1										X			X	
Octyl phenols	X	P/D		2										X			X	
Organotin compounds		D		2	2	2							X	X		X	X	
Pentachlorobenzene	X	D	3	3	3	3									X	X	X	
Pentachlorophenol (PCP)		D		3	3	3								X	X	(X)	X	
Perfluorocarbons (PFCs)		D	3							X								
Phenols		D/N		2										X				
Phosphorus, total		P/D/N		1				X										X
PM_{10} (Particulate matter less than 10 µm)		P/D/N	1								X							
Polychlorinated biphenyls (PCBs)	X	D	3	2	2	2									X		X	
Polycyclic Aromatic Hydrocarbons (PAH)		P/D/N	1	2	3	3					X			X	X		X	
Sulphur hexafluoride (SF_6)		D	3									X						
Sulphur oxides (SO_x)		P/D/N	1				X				X							
Tetrachloroethylene (PER)		D	3						X		X							
Tetrachloromethane (TCM)		D	3	2					X		X							
Toluene	X	P/D	2	3					X		X			X				
Total Organic Carbon (TOC)		P/D		1										X				
Toxaphene	X	D	3	3	3	3									X	(X)		
Tributyltin and compounds	X	D		2		2							X	X		X	X	
Trichlorobenzenes (TCBs)		P/D	3	3	3	3									X		X	
Trichloroethane-1,1,1 (TCE)		P/D	3	3	3				X		X							
Trichloroethylene (TRI)		P/D	3	3					X		X							
Trichloromethane (Chloroform)		P/D	3	2					X		X							
Trifluralin	X	D	3	3	3	3								X		X	X	

Table 36 Possible groupings of EPER and EPRTR substances — contd

			Monitoring data				Impacts and concerns											
Substance	**EPRTR substance**	**Sources**	Air	Water and sediment	Soil	Biota	Acidification	Eutrophication	O_3 formation	O_3 depletion	Local air pollution	Global warming	Heavy metals	Org water pollutant	POP or POP-like	Pesticide	Possible EDS	Inorg water pollution
See note No:	1	2	3	3	3	3	4	4	4	4	4	4	4	4	4	4	4/5	4
Triphenyltin and compounds	X	D		2		2							X	X		X	X	
Vinyl chloride	X	D	2	2							X							
Xylenes	X	P/D	2	3					X		X			X				
Zinc and its compounds		P/D/N	2	2	2	2					X		X					X

1. EPRTR substances. A 'X' in this column denotes that the chemical is listed in the proposed European Pollutant Release and Transfer Register. Substances not denoted by a 'X' are listed in both EPER and the proposed EPRTR.
2. Sources. The principal environmental sources of the substances are denoted as follows: P = mainly point sources from facilities listed in EPER, D=diffuse sources, such as vehicle emissions, agricultural chemicals released during or following application to land, releases from small industrial premises, releases during the life or disposal of products containing the substance in question. N = substances having significant natural sources.
3. Monitoring data availability. Monitoring programmes are largely driven by the need to demonstrate compliance with legislation. Therefore substances that are already extensively controlled are largely those with the most comprehensive sets of monitoring data available. Availability of monitoring data in air, water and sediment, soil and biota was assessed on a simple three point scale: 1 = good coverage of data; 2 = moderate data coverage and 3 = sparse data coverage.
4. Impacts and concerns. A 'X' in the relevant columns indicates that the substance is of concern because of particular environmental effects (acidification, eutrophication, etc.) or type of substance (heavy metal, pesticide, etc.). EDS = endocrine disrupting substance. (X) indicates a pesticide banned in the EU.
5. 'X' indicates that the substance (or a component of it if the 'substance' listed is a mixture of related chemicals) is suspected of interfering with the hormone systems of humans and wildlife and is listed as such in the EC Commission Staff Working Document SEC(2004)1372, or BKH report for the European Commission. Towards the establishment of a priority list of substances for further evaluation of their role in endocrine disruption: preparation of a candidate list of substances as a basis for priority setting. Final report, November 2000 (89).

The EEA website also lists several databases of European environmental monitoring data and other information is available at a national level. Sources of information on environmental concentrations of chemicals and other information useful for chemical modelling were given in Table 19. In addition, for a limited number of substances listed in EPER and the EPRTR there are also European Risk assessment Reports, either in draft or completed form, available from the European Chemicals Bureau, which provide information on environmental concentrations and exposure (Table 37).

Having developed a list of candidate chemicals and identified sources of information for screening modelling, the next step would be to identify, as far as possible, relevant environmental quality criteria against which the model outputs may be assessed. Depending on the nature of the predicted environmental concentration generated by EUSES modelling, this could be defined as an appropriate proportion of a relevant standard. It is anticipated that in many cases there will be no official environmental quality standards defined. In these cases, it would be appropriate to consider alternative approaches, such as the proportion of background concentration contributed by EPER sources. The rationale for the selection and development of these criteria would need to be clearly and transparently defined. As part of this step, consideration should be given to the issues of defining the degree of exceedences that can be accepted — i.e. a normative step. Comparison with the agreed defined standards would form the basis of deciding the need for further modelling.

On the basis of the work undertaken so far, the next step would be to finalise a shortlist of candidate substances for screening modelling, omitting any for which there is judged to be insufficient supporting data to make the analysis worthwhile. This list would be agreed before proceeding with the

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(89) http://europa.eu.int/comm/environment/docum/01262_en.htm#bkh. Category 1 chemicals from Annex 1: Candidate list of 553 substances: http://ec.europa.eu/environment/docum/pdf/bkh_annex_01.pdf.

modelling itself. Scripts would then be developed to run EUSES for each of the selected substances and to generate the required outputs. The results would then be evaluated against the defined criteria in order to identify the chemicals showing exceedances of the defined limits. Further modelling of these substances would then be undertaken in Task B.

Task B — Further EUSES modelling
Task B would involve further modelling with EUSES, in this case applying sector- and location specific factors to reduce the conservatism of the model outputs. In the case of emissions to air, this would include the use of sector-specific discharge height data to be applied to releases from all relevant facilities, or water flow or catchment data for chemicals released to water, and type of wastewater treatment. In the case of substances with multiple congeners such as dioxins, further analysis should be undertaken using the congener profiles typical of the relevant industrial sectors, where this information is available, to replace the worst-case assumption outlined in Task A. This part of the work would require identification of the key sectors and processes that contribute to the emissions of interest and then characterising the relevant release parameters so that these could be read into EUSES. For this stage of the work, geographical data characteristic of the location or region of each emitting facility will need to be identified and used in the analysis to replace the default values built into EUSES. Examples of regional-specific information would include river flows, temperature, rainfall, soil and vegetation cover, and so on. A rational strategy as to how this information should be presented to EUSES would need to be developed. Possible alternative approaches could include on a catchment basis, fixed matrix or flexible grid centred on each facility (as used in the model demonstration in this study). Alternative methods of presenting the results should be explored, as outlined in Section 4.2.2.

In order to identify sensitivities to variations in key input data, certain appropriate input parameters should be identified for further analysis, and allowed to vary within pre-set limits. This would involve providing EUSES with alternative values in order to explore the impact of variations in input data on the magnitude of predicted output concentrations and hence to identify which input parameters have the greatest overall effect on the output. This part of the analysis should be undertaken for a limited number of selected chemicals representing different types of environmental behaviour. Further analysis should also be undertaken to assess the uncertainty in modelled output concentrations, based on the Monte

Table 37 European risk assessment documents for EPER and EPRTR substances

Substance listed in EPER or EPRTR	Relevant European risk assessment reports
Benzene	Draft
Benzene, toluene, ethylbenzene, xylenes (as BTEX)	Draft available for benzene and toluene
Brominated diphenylethers	Completed for penta- and deca-bromo derivatives, draft available for penta-bromo
Cadmium and its compounds	Completed for oxide and cadmium metal
Chloro-alkanes (C10-13)	Draft
Chromium and its compounds	Drafts available for chromium trioxide, sodium chromate and dichromate, and ammonium and potassium dichromates
Fluorides	Draft for hydrogen fluoride
Fluorine and inorganic compounds (as hydrogen fluoride)	Draft for hydrogen fluoride
Naphthalene	Complete
Nonylphenol ethoxylates (NP/NPEs)	Completed for Nonylphenol (branched) only
Tetrachloroethylene (PER)	Draft
Toluene	Complete
Trichlorobenzenes (TCBs)	Complete for 1,2,4-trichlorobenzene
Trichloroethylene (TRI)	Complete
Zinc and its compounds	Complete for zinc chloride, distearate, phosphate, sulphate and zinc metal

Note: Risk assessment reports are those listed on the European Chemical Bureau's website on 7 September 2005. http://ecb.jrc.it/home.php?CONTENU=/DOCUMENTS/Existing-Chemicals/

Carlo analysis. This would entail running EUSES repeatedly for alternative values of input parameters sampled from predefined statistical distributions. The resulting distribution of output results would indicate the overall uncertainty in the analysis.

Having identified the strategy for sector and location specific EUSES modelling, the next step would be to modify the scripts to feed this information into the EUSES model. Having run EUSES with sector- and location specific input data, the results will then need to be compared with the relevant environmental criteria. For those releases for which there are no exceedances, no further analysis would be undertaken. However, additional detailed modelling would be required (in Phase 2) to enable the output to be used to predict Europe's chemical density from EPER emissions. An outline plan describing the proposed approach to detailed modelling will be developed in the light of this analysis, identifying the models to be used and as far as possible the input data requirements.

Task C — Phase 1 interim report
The results of the study so far would then be synthesised into a detailed interim report, describing all of the work undertaken in Tasks A and B, the methodology and rationale, results, conclusions and draft recommendations for the second phase of the work. The interim report would be discussed and reviewed at an expert workshop held as part of Task D.

Task D — Expert workshop
The key activity in Task D will be to organise an expert workshop to review the outcome of the work so far and in particular to comment on the approach proposed for further detailed modelling, as identified in the interim report. The workshop should include leading experts in the field of chemical modelling, together with other stakeholders. A key aspect would be to assist in the development of the detailed modelling strategy and to advise to input data availability.

Task E — Phase 1 final report
Following the workshop, the interim report will be revised and updated in the light of discussions, putting forward well-defined plans for completing the study in Phase 2, with detailed modelling. The draft final report would be reviewed, following which the final version would be produced. It is intended that the Phase 1 final report would contain all of the information, so as to decide whether to proceed with the second phase of the study.

4.3.2 Proposed Phase 2 outline work plan

The detailed work plan for Phase 2 of the work plan will be developed as the main output from the first phase of the work, so at this stage it is possible to make only general observations on type of tasks that Phase 2 will involve.

Clearly a major component will be the detailed modelling of selected substances, using temporally and spatially resolved models, selected according to the properties of the chemicals under consideration. It is expected that the models used will be sufficiently well-proven for use in a policy context, be appropriate for their intended use, and are expected to include models reviewed in the first part of this feasibility study. The modelling would need to be undertaken by experienced experts in the field, either using models commercially or freely available, or (if the models are not available to third parties) under contract with the model developers. Access to input datasets, such a meteorological, hydrological, geographical and land cover data will be required and this will need to be provided in a form compatible with the models' requirements. Some pre-processing of input emission data may also be needed, depending on the model resolution. For example, aggregation of sources may be required, depending on the spatial grid resolution of the model used. Combinations of models may also be required — for example, detailed air dispersion modelling of substances release to this medium, followed by multimedia media modelling where the substance has the persistence and ability to move between media, for example, in the case of some POPs. Obviously, the precise approach to such detailed modelling will depend on the substances selected and analysis undertaken in the first phase of the work.

To ensure scientific authority of the work, it is proposed that an expert workshop be held at a suitable stage in Phase 2 to review the findings and to promote the work to key stakeholders. As with the first phase, it is suggested that the workshop reviews the findings presented in a Phase 2 interim report. The final report would then incorporate feedback on this document in the light of the workshop discussions. The results of work should be made available on a project website that should be developed as part of Phase 2. However, this should be restricted to regional and greater scale modelling, and exclude local predicted concentrations.

4.4 Conclusions from Phase 2

The following conclusions are drawn from Phase 2 of this feasibility study:

1. Following the completion of the model evaluation undertaken in Phase 1 of this feasibility study, two options were identified for the strategic plan needed to predict the chemical density of Europe from emissions data. The options were: (1) a detailed modelling approach, and (2) a staged modelling approach, in which a screening model would be used to identify those emissions where further detailed modelling would be required. The staged modelling option is consistent with the tiered approach to modelling endorsed by the OECD for predicting the persistence and potential for long-range environmental transport of chemicals.
2. The study concluded that the second option (the staged approach) would offer the most cost-effective and efficient way forward. It makes use of an established multi-media screening model for initial analysis of environmental concentrations resulting from EPER emissions. Comparison of the environmental concentrations predicted by the screening model with relevant environmental standards or other appropriate criteria would then be used to decide on the need for further assessment with more complex models requiring detailed spatially and temporally resolved input data.
3. The staged approach that underpins the strategy offers the advantages of cost effectiveness by only undertaking detailed modelling in cases where regional exceedances are predicted by the screening model and no alternative information sources are available.
4. The EU chemical risk assessment model EUSES was identified as being suitable for undertaking the screening assessment as the first part of the staged modelling strategy and its use in this role has been demonstrated by application to emissions of three contrasting chemicals listed in the EPER database. The chemicals were hexachlorobenzene, benzene and arsenic.
5. Scripts were written extract emission data from EPER and to run EUSES with each substance in turn and to generate map outputs of predicted local and regional environmental concentrations in air, surface water and (for arsenic) soil, allowing 'hot spots' to be identified.
6. The suitability of the EPER database as a source of data for concentration modelling has been assessed. The database allows information to be extracted readily to provide the input to chemical fate models by means of simple computer scripts. The database gives details of the geographical location of each source and so it is relatively straightforward to prepare maps of pollutant hot spots associated with EPER sources. The provision of the details of the geographical location of the site also greatly facilitates the extraction of site-specific environmental data for modelling from climate, land cover and river catchment databases.
7. To some extent, the EPER database duplicates the information already held in the EMEP large point source inventory. However, the EPER database provides information on emissions of a wider range of pollutants to both air and water; will be updated more frequently and includes a wider range of sources.
8. The EMEP large point source database provides information on the height of discharge above ground: this element is not available from the EPER database. It would be useful for the calculation of local and regional air concentrations, which are dependent on the height of emission.
9. We have considered whether the EPER data provides added value for both high and low resolution assessments. Our experience with hexachlorobenzene, benzene and arsenic modelling suggests that the EPER database does not contain sufficient information to allow a high-resolution detailed assessment to be carried out. For example, a detailed local assessment of air dispersion would require additional information about discharge stack heights and diameters, the temperature and velocity of discharge and local topographical details. In addition, detailed information on the composition of several chemicals that are reported as mixtures of related species is lacking. The format of the data is however suited to low resolution-screening assessments of large numbers of sources.
10. EPER may increase the usefulness of existing models on the (pan) European and regional level because it contains data for many more point sources than the existing data sources. Currently, it is often necessary to spatially disaggregate national or regional emission totals onto an emissions grid for modelling purposes. The EPER data will allow more precise allocation of emissions onto the model grid.

11. A simple addition to the EPER data return form is proposed that would allow information on local environmental concentrations to be submitted has been developed.
12. A draft work plan has been prepared to predict the chemical density of Europe from emissions of other substances listed in EPER. The first phase of this work, which would require two stages of EUSES screening modelling of selected substances, identification of appropriate assessment criteria and sensitivity and uncertainty analysis, is estimated to require about 80 man-days effort. The second phase would involve detailed spatially resolved modelling of substances found to exceed the relevant criteria in the first phase. Because of difficulties in gaining access to site-specific information needed to undertake accurate modelling of environmental concentrations, it is recommended that the assessment focus on modelling at the regional or greater geographical scale, rather than the local scale.
13. Overall, we believe that the staged proposed in this study will provide a feasible, cost-effective and efficient means of predicting the chemical density of Europe from industrial point-source emissions data. Further work would be required to predict chemical concentrations resulting from non-point sources, which in many cases are the dominant source of environmental releases, but where information on emission rates is currently much less available.

Appendix 1: Technical specification

A1.1 Introduction

A1.1.1 Background

Chemical substances that are present in the environment may cause negative impacts not only on environmental sectors but also in humans. Adequate knowledge about substance concentrations in environmental media is an absolute requirement for any reliable assessment of these impacts and risks.

Although monitoring is already conducted under several voluntary and legal schemes the process of risk assessment under the existing substances regulation 793/93 highlighted a general lack of knowledge on the exposure to the existing substances under review. To improve this situation, EEA has given a high priority to the development of a monitoring framework to provide data to build the basis for better assessments that also allow following the effects of policies and measures.

However the high number of chemicals on the European market does not allow monitoring all of them. Modelling of their distributions could be used to supplement the picture.

The aim of this feasibility study is to explore the availability of suitable models to predict environmental concentration of chemicals from point source emission data such as the data reported to EPER and develop a strategy how these can be used to assess the chemical burden of Europe's environment.

EPER is the European pollutant emission register EPER http://www.eper.cec.eu.int/ — the first European-wide register of industrial emissions into air and water. It gives access to information on the annual emissions of 9 376 industrial facilities in the 15 Member States of the EU as well as Norway and Hungary — mostly from the year 2001. The EPER database does contain release data on about 50 substances. Models might be applied to predict the distribution of these substances following their release. Available monitoring data may be used to verify model estimates.

A1.1.2 Previous work

The EMEP-programme under the convention on Long-range Transboundary Air pollution (LRTAP) http://www.emep.int regularly provides information on concentrations of POPs based on monitored and modelled data.

Several research programmes from public site and industry have been active in the development of models, e.g. GREATER. The Technical Guidance Document (TGD) on Risk assessment of chemical substances1 ([90]) provides information on exposure models used in the risk assessment process (e.g. the European Union system for the Evaluation of Substances EUSES, for details see http://ecb.jrc.it/existing-chemicals/). The OECD maintains a web based inventory on a number of models useful for chemicals assessments i.e. distribution models.

EEA is carrying out a specific project with the scope to identify, assess and map the areas that present soil contamination problems to be dealt with at the European level. The project is a direct contribution to the preparation of soil monitoring guidelines under the Soil Thematic Strategy (STS) and a support to assessment and reporting activities. To this scope a risk-based approach has been adopted. The methodology developed makes use of Europe-wide geo-referenced databases such as EPER and DECHMINUE (mining waste data). The expected outcomes of the project are:

- a proposed method for the identification of areas under risk of soil contamination in Europe;
- a map and related assessment focusing on soil contamination risk areas, produced by applying the proposed method ([91]).

([90]) The Technical Guidance Document in support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market.

([91]) Background documentation is available under http://eea.eionet.europa.eu/Members/irc/eionet-circle/te/library?l=/eionet_contaminated&vm=detailed&sb=Title ; publication of of the results as EEA working paper is under preparation: EEA, 2007. Towards a EEA Europe-wide assessment of areas under risk for soil contamination — Final report (working title).

Activities of other international organisations in the development and application of modelling are also important and shall be considered in the investigation. This includes programmes of EU, WHO, UNECE, OECD.

A1.2 Purpose of study

Develop a toolbox of available methodologies and a work plan for applying relevant models to substances reported under EPER in order to predict the concentrations, composition and distribution of these chemicals in the European environment.

The main task in this feasibility study will be to:

1. evaluate

- which of the available methods to model environmental concentrations of chemicals in the different media are sufficiently validated and accepted to be used in a policy context;
- which of the models are suitable for all or some of the substances listed under EPER and other types of compounds.

2. make a test run; and
3. develop a strategic proposal how these models and derived data can be used to estimate and predict the concentrations, composition and distribution of chemicals in the European and wider environment based on European emission data.

A1.3 Tasks

The tasks to be performed are:

1. Identify available models on chemical substances concentrations in the different media and/or their impacts. The evaluation shall cover models to predict concentrations in air, water, sediment and soil as well as biota (excl. food). International and national developments should be considered as well as research activities especially those concerning persistent substances or substances with a potential for long-range transport, or activities covering large rivers or other areas which might be representative for particular European regions.
2. Verify their status of validation and general acceptance.
3. Evaluate available environmental models, preferably validated or widely accepted models, for their ability to provide information on spatial distribution of chemicals and resulting concentrations in different environmental media. Although the main target is Europe, regions outside Europe that will be impacted by European emissions should be included in the assessment.
4. Scan the models and provide information on the time and spatial scale they are able to cover. Provide expert judgement on the resolution needed for assessments of (pan) European, national, regional or local pollution. Describe model characteristics relevant for each of these levels.
5. Identify which of the above models are applicable to EPER substances.
6. Run one ore more selected readily available models for one or more test substances by using the reported release data in the EPER database. In selection of the test substance(s) consider the availability of monitoring data on the compound(s) as a key requirement.
    - Map the concentrations;
    - Identify hot spots of predicted high chemicals concentrations;
    - Assess usefulness of EPER data format for this purpose. For substances already covered by EMEP: discuss the added value by using EPER data for high and smaller resolution assessments. Will EPER data increase the usefulness of existing models on pan-European, regional, or local level?
    - Compare predicted levels with actual monitoring data on concentrations, if available.
7. Draft a work plan on how to extend Task 6 to all the relevant models identified in Task 5 and all substances reported in EPER. Define the minimum and optimum input parameters for the models needed to include further priority substances. Consider how substances could be grouped according to similar environmental effects, availability of monitoring data, expected releases (only point sources or many diffuse sources). Provide an estimate of the timeframe and required resources for executing the work plan.

8. Develop a strategic proposal on how these models and derived data can be used to estimate and predict the 'chemical density' (concentrations, composition and distribution of chemical substances) in the European environment based on emission data. Give an estimate of the reliability and level of uncertainty.
9. Summarise the findings of the feasibility study in a report.

A1.4 Geographic coverage

The ultimate goal is to develop an approach that covers the 31 EEA member countries, the six collaborating countries (Albania, Bosnia-Herzegovina, Croatia, Former Yugolav Republic of Macedonia, Monaco, Serbia-Montenegro) and Switzerland (92). The current EPER data covers emission sources in EU-15, Norway and Hungary. Within the frame of the feasibility study however high quality models should not be excluded because the geographic coverage is not complete. There should however be a description of the prerequisites to extend their applicability. Areas outside Europe that are impacted by European emissions should also be included in the considerations.

at the start of the project and submitted at least one week before the start-up meeting for approval by the EEA project manager. There are no special requirements regarding the location of work. It is envisaged that three meetings with the EEA project manager will be necessary:

A1.5 Deliverables

The consultant should submit the following deliverables:

1. Detailed work plan for the project, one week before the start-up meeting (three hard-copies and one Word file).
2. Inception report after the start-up meeting.
3. Interim report approximately two months into the project: overview on available distribution models, their status of validation, applicability and required input parameters (three hard-copies and one Word file).
4. A report with an analysis of the feasibility to use certain models to evaluate the geographic distribution and environmental concentrations of chemicals. The report shall provide an outline and detailed planning for such an assessment.

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(92) At the time of the study, Switzerland was not a member of the EEA. Switzerland became a member on 1 April 2006.

Appendix 2: List of participants

Delegates to the brainstorming meeting held at AEA Technology's offices at Harwell International Business Centre, Didcot, Oxfordshire, United Kingdom, on 2 March 2005

Name	Affiliation
John Abbott	AEA
Martin Adams	AEA
Keith Brown	AEA
James Cadman	AEA
Ian Bristow	AEA
John Stedman	AEA
Peter Coleman	AEA
Jenny Corps	AEA
Alberto Pistocchi	JRC
Mike Holland	EMRC
Joseph Spadaro	Centre d'Energétique of the Ecole des Mines de Paris
Helen Wilkinson	Environment Agency
Maarten van Loon	MSC West/Norwegian Meteorological Institute
Ian Whitwell	Environment Agency
Gabriele Schöning	European Environment Agency
Andreas Barkman	European Environment Agency
Ivan Holoubek	TOCOEN
Martin Holt	ECOTOC
Michael Whelan	Unilever
Andrew Riddle	AstraZeneca
Pete Roberts	Shell Global Solutions

Appendix 3: Comments on the draft final report from experts at the Brno chemical modelling summer school, July 2005

(With annotations on the project team's response)

Michael McLachlan, Stockholm University, Sweden:

General comments
I think that the report is well written and that the strategy adopted is in general good!

I have a few specific comments listed below.

Review of the multimedia models
The review does not adequately address the key issue of steady state/non-steady state. Steady state models will not perform well for chemicals with an environmental elimination rate that is comparable or longer than the time scale being modelled (e.g. one year). A considerable number of the chemicals in the EPER database are quite persistent. Using a steady state model such as EUSES will be conservative in this regard, and thus the proposed strategy is ok. However, these models will not be appropriate for higher tier assessment e.g. reconciling model predictions with measured concentrations. Furthermore, for persistent chemicals non-steady state models should have a key role in higher tier risk assessment, as monitoring will only give a snap shot. The future development of the environmental concentrations can only be evaluated with a non-steady state model.

Response: *Agree — for persistent chemicals, non-steady state models will be needed, but under the step-wise strategy proposed in the report, this detailed modelling would only be required where the EUSES screening indicates that relevant thresholds may be exceeded.*

There may also be some limitations to using the standard EUSES parameterization. As I recall (and I may be wrong) the standard parameterization has almost no water (5 %?). On the other hand, many of the population centres and industries are located in coastal areas. For chemicals emitted to air that are retained in the terrestrial environment but potentially harmful in the aquatic environment, EUSES will not be conservative.

Response: *The report acknowledges the potential for making EUSES parameters more relevant to the location and characteristics of the emission. We will re-emphasise this point.*

The classification of the models is not always correct. For instance, ChemCan and ChemFrance are spatially resolved multimedia models.

Response: *Good point — we will check this out and revise accordingly.*

CoZMo-POP is not a level I, II or III model (p.47), it is level IV. Furthermore, a second version has been released (check Frank Wania's website http://www.scar.utoronto.ca/~wania/). The justification for discarding this model is not clear, as CoZMo-POP has flexible landscape parameters, and as a level IV model it is more flexible than the level III models listed. The context of the statement 'the final report is expected in 2005' (p.48, par. 1) is not clear. Also, I am not sure that Frank Wania would agree with the description of the motivation for developing the model.

Response: *We will check these points and revise as appropriate.*

Gerhard Lammel, Max Planck Institute, Hamburg, Germany:

1. Emission data of organic chemicals, e.g. as reported by signatory states to the UNECE CLRTAP under the POPs Protocol or based on expert estimates, are considered to be very uncertain and vary between substances. One order of magnitude is typical but not a worst case. The mode of entry (split among receptor compartments) is unknown for many relevant substances (implicitly acknowledged e.g. in Section 4.2.2). The compartmental distribution as predicted by multimedia models (levels III and IV), however, is strongly influenced by the mode of entry.

Response: *Not sure what, if any, revision the reviewer is suggesting here. We agree that the mode of entry strongly influences compartmental distribution and will ensure that this point is clearly made in the next issue.*

2. Region-specific models should be capable to account for the variety of significant mass transfer and partition coefficients in the region and for advection from the boundaries of the region. Partitioning of non-polar organic substances between water and air is influenced by more processes than covered in the models. Partitioning between soil and air is influenced by partly unknown features of soil texture and physical and chemical state of soil not covered in multimedia models. Partitioning between vegetation and air is dependent on plant species / plant physiology, only partly understood and not yet covered in the models. Therefore, predicted compartmental distribution may both overestimate and underestimate compartmental burdens. For some substances, the description of the boundary conditions needs nested or global-scale modelling.

Response: *We will revise the report to state that there are many other processes influencing the distribution of non polar substances that are not well-addressed in current models.*

I cannot comment on respective deficiencies with regard to other than non-polar organic substances.

3. A screening model to be used in a staged approach (Section 4.1.1) should guarantee conservatism (exclude underestimates). Due to the abovementioned (2) and various other reasons (e.g. no fast atmospheric transport as frequently happening in the boundary layer and even more so aloft is reflected in EUSES), no such model exists. Even the decision tool can guarantee conservatism, any tiered approach as suggested obviously implies a normative step, namely the choice of a tolerable amount (or fraction) of undetected underestimates (hence, possible exceedances) in both temporal and spatial dimensions, not mentioned in the draft.

Response: *We agree that there will always be a risk that a screening model will give a false negative. Setting the acceptance criteria to give an appropriate margin of safety may reduce the chances of this happening. This is an important issue but one that needs following up in later work, rather than forming part of the present feasibility study. The potential for this issue being a practical problem will become more apparent when the results of screening a wider selection of chemicals has been undertaken.*

4. Some minor points: Chapter 3.3 names the Hysplit4 and CMAQ models which, however, are not multimedia models but atmospheric models. 'Kloepffer' should read 'Klöpffer'. The acronym IPPC should be introduced at the first place where it's used (in the Executive Summary).

Response: *OK — these points will be addressed in the next issue.*

My (preliminary) conclusion would be that:

An *a priori* decision about tolerable fractions of undetected underestimates in time and space is needed.

Response: *See above*

The conservatism of screening models should be validated, e.g. by comparison of screening model output against temporally and spatially high-resolved observation data and geo-referenced model output, the latter in order to capture the non-linearities caused by averaging over inadequate ranges of time and space, the entire model domain and the uncertainties related to mode of entry.

Response: *This has already been done for arsenic in the present report — see Section 4.2.4.*

Detailed regional modelling, in a higher tier, should be done using coupled models of atmosphere, water and soil. These should be improved to minimize abovementioned deficiencies (2).

Response: *This would be a sensible way forward IF the screening approach with EUSES indicates that there is cause for concern. Coupled models could well be a way forward, but would be extremely resource-intensive for use as the first stage, and (as much of the required input data are not available) would not be possible. Coupled models may not be appropriate for chemicals where there is little intermedia transport, so we cannot make this generalization.*

Victor Shatalov, MSC-East Moscow, Russia:
The EMEP models are not currently available for use outside MSC-East since a lot of input data is required (meteorology, land cover, etc.). In future some form of the models may become available. The models can be run on PCs. It may be possible for the EEA to negotiate….

Response: *OK — these points will be addressed in the next issue.*

Johannes Ranke, University of Bremen, Germany: Although my review includes some points of criticism, I must stress that I found the collection of models useful and interesting.

Two comments to the 'Attributes of an ideal model toolbox'

Applications:

– Tools are required that will allow EPER emissions to be used, with appropriate supporting data, to predicted environmental concentrations of chemicals.

Spelling mistake: 'predicted' should read 'predict'.

Response: *OK.*

Scientific validity:

– Well-proven models with an established record of use will be preferred over novel but perhaps less proven approaches.

This argument is foggy. If a novel model is less proven, this of course is a strong argument against it. If, a novel model is equally or even better proven, the established record of an older model should not lead to its preference in my opinion.

Response: *We'll think how to rephrase this. However, the fact remains that proven models should be preferred to novel models for the purpose under consideration. 'Novel' models will not, of course, be as well-proven as more established models, but as they build up their record of successful validated application, then they will in turn become 'well proven'.*

Model description section: Why were three types of air quality models, surface water models and sewage treatment plant models included in the review, when a multimedia model was sought, as it appears?

Response: *Because this was what we were asked to do. If we/EEA knew what the outcome of the work would be when the contract was tendered, there would have been little point in doing the work!*

First paragraph of the section called 'Application of screening models to EPER emission data' within the description of the EUSES model.

Several of the models discussed above could be suitable for predicting environmental concentrations at local, regional and continental scale of chemicals released from industrial sources, such as those listed in EPER. However, EUSES would appear to be the obvious choice for such application, given that it has been designed specifically to fulfil the requirements of the EC Technical Guidance Documents on chemical risk assessment, it has been extensively peer-reviewed and is the widely-accepted tool in the EU for chemical risk assessment. This stands it in good stead to be used for the related application of assessing concentrations from point-source releases.

It appears to me that this reveals some preconceptions that the authors have about the 'natural' choice of the model, just at the beginning of the discussion of multimedia models, merely based on the official status of the EUSES model.

One might argue, on the contrary, that the fate model within the EUSES expert system is many years old nowadays, some alternative models have evolved substantially in this time, while the official status of EUSES effectively excluded it from such progress to a large degree.

The necessity to adapt the EUSES model parameters from 'reasonable worst case' to 'reasonable average case' which would be necessary is another argument against using EUSES outside of its dedicated purpose, being the risk analysis of chemicals.

Response: *We accept that EUSES is not perfect, but that does not exclude it from its proposed use as the first step in the strategy proposed. How much harder it would be to justify a non-well established alternative model in this role, given the interest that publishing estimated environmental concentrations on the Internet will attract. There is no reason to go to ever more complex models if the data needed to drive them are not available. This is why we advocate the staged approach. If the screening with EUSES suggests that there may be cause for concern, the public availability of this information will help motivate those with access to the best local data (ie industry and regulators) to make it available. If EUSES indicates that there could be regional concerns, then the relevant authorities will need to devise a detailed modeling / monitoring study to investigate them further. The alternative approach of going straight to detailed modelling would be very resource-intensive and unnecessary for many emissions.*

Evaluation of the EMEP model:

In considering the EMEP output data, it is important to remember that the predicted geographical distributions are entirely based on computer modelling and have not been verified by measurements made on a comparable geographical basis. The main driver for the predicted concentrations is the emission data and inaccuracies in this key input data will be reflected in the output obtained. Much of the input emission data for the source grid are based on 'expert judgement' and consequently the outputs, too, reflect this judgement.

There are a couple of remarks that I would like to make regarding this paragraph. The first statement is not true. V. Shatalov, one of the main authors of the model, has presented comparisons of model results with measured data and has shown agreement.

Response: *OK — perhaps this is a little harshly worded. However, the point remains that modelling results are largely unverified by monitoring on a comparable geographical basis.*

The second statement is obviously valid for any model that will predict concentrations from emission data. It should not influence the evaluation of the model.

Response: *It doesn't.*

The third statement seems to me to be irrelevant in a similar manner, since all models use expert judgment, be it for allocation or estimation of input data or for other purposes. In addition, I think putting the term 'expert judgment' in quotes is implicitly questioning the expert status of the authors and operators of EMEP in a to my mind somewhat impolite manner.

Response: *The fact that models rely on the subjective views of fallible human beings where input data are lacking seems to me to be highly germane as to how we evaluate the conclusions drawn from their outputs, and is not something we should be shy about. I cannot think of a single scientific advance that has not overturned the views of accepted 'experts' of their day. The quotation marks were not intended to question the quality of the judgment of these particular expert, but to avoid any suggestion that this was so, we will remove the offending punctuation.*

Computer resources needed for EMEP: On page 81 it is stated that a parallel processing supercomputer has to be used — in fact, according to V. Shatalov, AMD Athlon 64 based normal consumer PCs are being used.

Response: *We'll correct this in the next issue.*

Summary of part I, point 5:

... It is important to note that highly detailed models will not provide greater accuracy of output than a simpler screening model unless the input data is characterized with the required degree of certainty.

If, however, point sources are being considered, the exact location of the point source is known, and in such a case, it is crucial to incorporate basic meteorological input including main wind directions and speed. This is missing in EUSES.

Response: *And also missing in EPER is stack height data. Having met data without stack height would not be particularly useful, were we not using a staged approach with EUSES as the first stage. However, all this additional information would be needed for detailed modeling if the screening results from EUSES were to show that detailed modelling is required.*

Part II:

Since the strategy which is being proposed in Part II is based on the decision that the EUSES fate model is the tool best fitted to the purpose, I would argue that it would be necessary to devise an alternative strategy based on a spatially resolved model with meteorological input data. EUSES is a good tool for doing risk analysis for a generic region. If specific point sources are to be evaluated in terms of their contribution to concentrations in their regional environment, my feeling is that a model incorporating such important factors as wind directions and speed would perform significantly better. It might require some more institutional investments, but the gain would be significant in my opinion.

Response: *We agree with this comment, but the considerable resources needed for detailed modeling should only be deployed if the initial screening advocated in the strategy indicates that there is some need for better estimates. The advantages of the strategy are that it helps to focus attention on chemicals that may exceed relevant thresholds, it will stimulate industry (and regulators) who have the best knowledge of local concentrations to provide missing data to overwrite the screening model predictions and help identify substances where detailed regional scale models may need to be deployed. It is not a way of avoiding detailed modelling — just a way of focusing on where it may be most cost-effectively applied.*

Finally — Ivan Holoubek — I discussed these remarks mentioned above and I agree with the authors. My remarks were included to their as a results of our discussion.

Appendix 4: Proceedings of expert workshop, 16 August 2005, EEA, Copenhagen

See separate document.

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