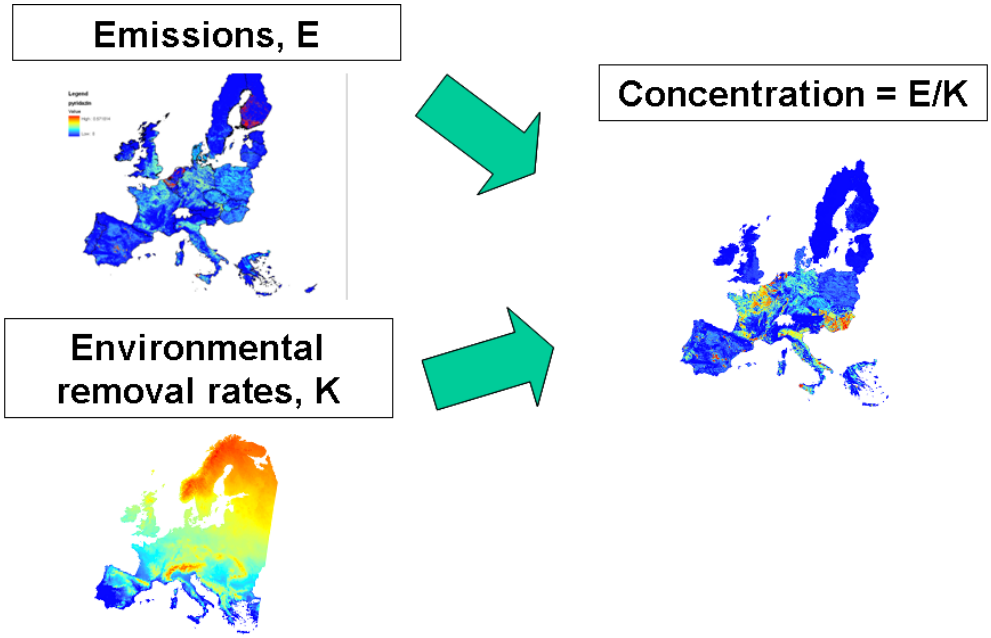
JRC Scientific and Technical Reports

An assessment of three priority hazardous substances at the European scale

Alberto Pistocchi, Pilar Vizcaino, Robert Loos



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Contact information
Address: Alberto Pistocchi, JRC, TP 460, Via Fermi 2749, 21027 Ispra (VA), Italy
E-mail: alberto.pistocchi@jrc.ec.europa.eu
Tel.: 00 39 0332 785591
Fax: 00 39 0332 785601

http://ies.jrc.ec.europa.eu/
http://www.jrc.ec.europa.eu/

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1. Introduction - Objectives of the report

Within the European Union there has been concern for very long time about the usage and potential risks of chemical substances. The discovery that chemicals, once entered the environment, may persist and bioaccumulate in humans and ecosystems, or that they can form metabolites having potentially harmful effects, has lead to the adoption of a number of monitoring, risk management and control policies.
The aim of this contribution is to illustrate the state of knowledge about present loads of persistent priority hazardous substances to European marine waters via riverine discharge. As a follow-up, three representative substances will be selected for which a detailed assessment has been conducted.
In particular, maps of emission for three selected substances are provided, to the extent made possible by existing information, and the associated loads computed.
There is a knowledge gap on the occurrence of priority hazardous substances, and relatively little information is available. For instance, the Helsinki Commission (HELCOM) states:"The information currently available on inputs and sources of hazardous substances is not as extensive as for nutrients, so it is not yet possible to conduct a comprehensive assessment of the situation in the Baltic Sea. The HELCOM countries have therefore decided to work together to build up more information about the sources of the selected hazardous substances, the extent of their occurrence in the Baltic marine environment, as well as about their biological effects. This knowledge can then be used as a basis for identifying further actions."1
Information and legislation on priority hazardous substances is evolving. The material presented in this report is updated to December 2008 for what concerns background information and the selection of the study chemicals, and December 2009 for what concerns the case studies on three selected substances.

2. Existing legislation requiring the assessment of chemical pollution

Currently there are a number of legislative tools in the European Union concerning the regulation of chemical pollution in water. In this paragraph, we summarize the existing tools insofar as they set a framework for the acquisition of information on chemicals, potentially usable for chemical assessment.

2.1 Former risk assessment reports and REACH

The procedure for registration, evaluation, authorization of chemicals has come into force in the European Union in 2008, following regulation EC 1907/2006. The procedure applies to all chemicals excluding those for which an equivalent procedure already exists. Among these, pesticides and biocides are the main chemical classes containing potentially hazardous substances which are emitted to the environment. The REACH

[1] HELCOM web site: http://www.helcom.fi/press_office/news_helcom/en_GB/BSAP_Summary/?u4.highlight=hazardous%20chemical ; last accessed 7/29/2008

procedure calls for risk assessment of substances whenever applicable, and is expected to trigger a massive collection of data which will be available in the future.
At present, there are a number of chemicals already subjected to risk assessment according to the pre-reach legislation; some chemicals are already acknowledged to lead to undesirable effects and their environmental concentrations need to be under control. The outcomes of the risk assessment are provided through risk assessment reports (RARs) referred to individual substances or groups of substances. At present, risk assessment reports (draft or finalized) are available for 141 chemicals. These reports represent a comprehensive overview of the knowledge available about the production, fate, and effects of the target chemicals.

2.2 WFD and related legislation

The Water Framework Directive (WFD), 60/2000/EC, states that the European Commission proposes a list of priority substances, to be subjected to reduction and phasing out depending on their hazardous character. Moreover, member states are due to identify specific chemicals hampering the obtainment of good ecological status in water bodies of their river basins, within the cotext of river basin management plans. An indicative list of the main pollutants (annex VIII of the WFD) include Organohalogen compounds, Organophosphorous compounds, Organotin compounds, carcinogenic or other harmful substances, Persistent hydrocarbons and persistent and bioaccumulable organic toxic substances, Cyanides, Metals and their compounds, Arsenic and its compounds, Biocides and plant protection products, Materials in suspension, Substances which contribute to eutrophication (in particular, nitrates and phosphates), Substances which have an unfavourable influence on the oxygen balance (and can be measured using parameters such as BOD, COD, etc.).
The earlier directive 76/464 (codified as 2006/11/EC) requires that the member states adopt legislation to eliminate pollution from "list I chemicals" (i.e. organohalogen, organophosphorus, organotin compounds, substances proven to be carcinogenic, mercury, cadmium, persistent mineral oils and hydrocarbons of petroleum origin, persistent synthetic substances which may float and remain in suspension and interfere with any use of waters), and to significantly reduce pollution from "list II chemicals" (a number of metals, biocides, substances having effects such as smell and bad taste, toxic or persistent compounds of silicon, phosphorus, cyanides, fluorides, ammonia, nitrites).
A number of "daughter directives" have been adopted for the implementation of directive 75/464.
As of 2013, when Member states will have adopted appropriate measures for "annex VIII" and similar chemicals, the directive will be eventually repealed.

2.3 Pesticides and biocides

Pesticides are subject to authorization in Europe according to Council Directive 91/414/EEC. This directive sets a framework for risk assessment of pesticides for their placement on the market. Within this context, however, no specific monitoring is published that helps describing the situation in Europe. Technical reports are available for a limited number of substances already subjected to evaluation. These reports are similar to the RARs for chemicals now disciplined by REACH. A similar consideration holds for the biocidal products Directive 98/8/EC.

2.4 IPPC directive and EPER

The IPPC directive (Council Directive 96/61/EC, now codified in 2008/1/EC) sets a framework for the regulation of industrial emissions from industries of energy, metal production and processing, minerals, chemicals, waste management, pulp and paper, textiles, food, intensive rearing of poultry and pigs, surface treatment, and carbon production. Installations in the above categories are required to submit an application for permits which is similar to an environmental impact study. Among other obligations, the installations are required to report on emissions from a list of 50 chemicals, if their emissions are above a given threshold. Chemicals to be reported, and respective parameters are set in a 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)". At present, two years of reporting (2001 and 2004) are available. The reported emission data are available on-line with the European Pollution Emission Register (EPER). Although limited to the chemicals, industrial activities and thresholds specified in the Commission decision, this register is a first example of industrial chemical emission inventorying in the European Union. From the year of reporting 2007, EPER is foreseen to be replaced by a European Pollutant Release and Transfer Register (E-PRTR).

2.5 Marine Framework Directive and marine conventions

In line with the WFD, the Marine Framework Directive extends the goals of "good environmental status" to the marine environment. Explicit reference is made to the control of chemical pollution, but no specific measures are foreseen beyond what already contained in the WFD and in the Regional Sea Conventions (Baltic - HELCOM, North sea and Atlantic - OSPAR, Mediterranean - MEDPOL, Balck Sea - BSC), which are explicitly recalled in the Directive. Of the regional sea conventions existing in Europe, only HELCOM and OSPAR have so far produced lists of substances of priority action or attention for the respects of chemical pollution. For these substances, the member states of the conventions are expected to take actions to reduce or eliminate pollution. The approach is similar to the one of the WFD and pre-existing European legislation on chemical pollution of waters.

2.6 Persistent Organic Pollutants (POPs)

Persistent organic pollutants (POPs) are addressed at present through a number of conventions. The Convention on Long-range Transboundary Air Pollution (LRTAP), signed in 1979, "one of the central means for protection of our environment […], establishes a broad framework for co-operative action on reducing the impact of air pollution and sets up a process for negotiating concrete measures to control emissions of air pollutants through legally binding protocols."2 One such protocol is the one signed in Aarhus in 1998, concerning 16 persistent organic pollutants, namely: DDT, Dieldrin , Endrin, Aldrin, Chlordane, Chlordecone, Heptachlor, Hexabromobiphenyl,

[2] From the introduction to the EMEP web site: http://www.emep.int/ ; last accessed November 2008

Hexachlorobenzene, Mirex, PCBs, Toxaphene, HCH (alpha, beta, gamma), PCDDs, PCDFs, PAH.
The Stockholm convention on POPs involves more countries than the LRTAP Convention and presently covers 12 chemicals considered as worst offenders, also known as the "dirty dozen", all included in the Aarhus protocol: aldrin, chlordane, DDT, dieldrin, endrin, heptachlor, mirex, toxaphene, hexachlorobenzene, the polychlorinated biphenyl (PCB) group; dioxins and furans. The Stockholm convention provides also a structured context for the management of other ("emerging") POPs, so that the initial list of 12 chemicals is in expansion. At present, "candidate POPs" include all the ones under LRTAP not yet included in the Stockholm convention, plus: Pentabromodiphenyl ether, Octabromodiphenyl ether, PFOS, Pentachlorobenzene, Short-chained chlorinated paraffins, Endosulfan, Hexabromocyclododecane (HBCDD).

2.7 Monitoring data

At present, there is no unique database collecting monitoring data for WFD priority substances. A massive effort has been spent during the preparation of the priority substance list, in producing a database called COMMPS, which reflects monitoring in a number of European countries. Details on the database are provided on the web site: http://ec.europa.eu/environment/water/water-framework/preparation_priority_list.htm .
The COMMPS database is a collection of water and sediment data which helps providing an order of magnitude of concentrations or possible pollution levels in Europe. However, it is rather inhomogeneous in time and space, and has a very diverse degree of coverage for the substances. Figure 1 provides an indication on the abundance of measurements in COMMPS.

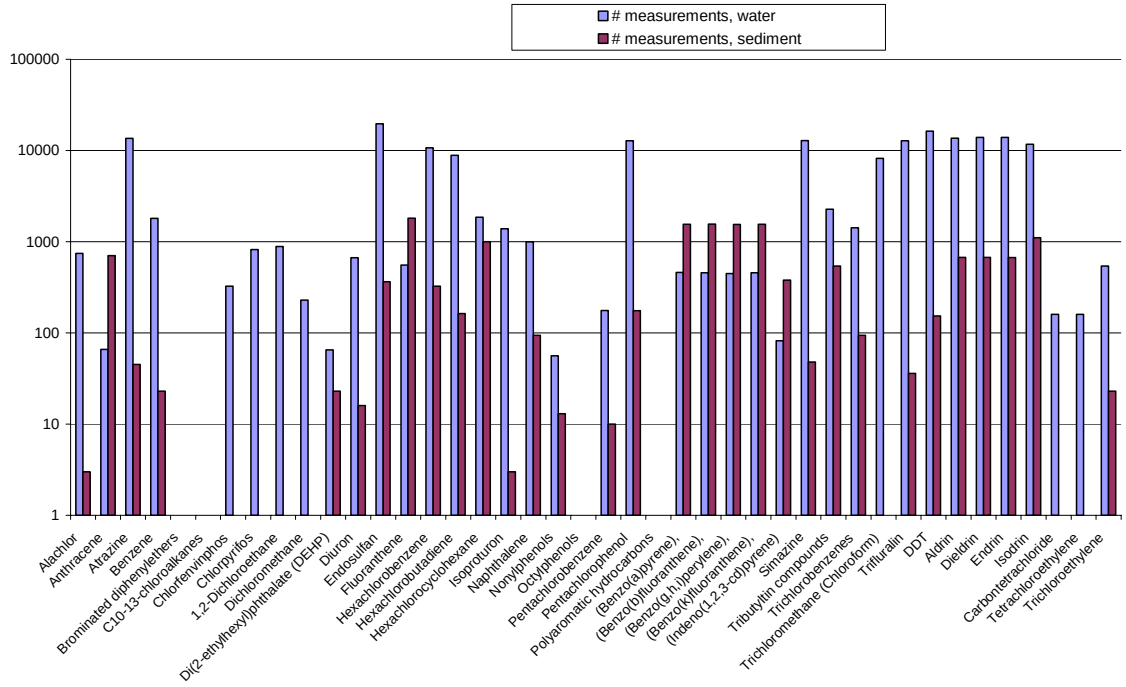


Figure 1 – Water and sediment monitoring data in COMMPS

Within Working Group E of the Common Implementation Strategy of the WFD, monitoring data on priority substances are being collected and structured in order to update the COMMPS list and database.

The EEA Waterbase is a database of water monitoring stations covering the whole EU. At present, only a few data are available for chemical pollutants, namely simazine, atrazine and lindane in groundwater.
(http://dataservice.eea.europa.eu/dataservice/metadetails.asp?id=1040)
For surface water (http://dataservice.eea.europa.eu/dataservice/metadetails.asp?id=1038), neither priority substances nor other chemical pollutants are included.

Monitoring of atmospheric concentration and deposition of the main "airborne" pollutants such as ozone, NOx, SOx, or PM is performed on a routine basis at the EMEP stations (www.emep.int). These stations provide also some information on the POPs of interest for the LRTAP convention.

The NORMAN project, funded by the European Commission within FP6, http://www.norman-network.net/index_php.php?module=public/about_us/home, aims at establishing and maintaining a database on emerging pollutants many of which are of concern as future priority substances for coastal areas. However, the database is still under development and does not warrant a systematic usability for model evaluation at present.

The European Environment Agency (EEA) is collecting data from the national monitoring programmes of the Member States, within the WFD activities. Reported data for chemical pollutants are available through the Central Data Repository of EIONET (http://cdr.eionet.europa.eu/), for individual Countries.

Monitoring of chemicals in marine waters is actively undertaken within marine conventions such as OSPAR and HELCOM. However, at present, data are available to the public only as summarized in reports.

HELCOM conducts a combined monitoring programme concerning both biota and seawater. Monitored substances (total concentration in seawater) include DDT and metabolites, CBs (Nos. 28, 52, 101, 118, 138, 153, and 180), hexachlorobenzene (HCB), PAH, alpha-, beta-, and gamma-hexachlorocyclohaxane (HCH). The Baltic sea monitoring stations are shown in Figure 2.

Monitoring programmes from individual countries of the Helsinki Convention cover more substances. In particular, the chemicals in Table 1 are foreseen to undergo monitoring in sea water by individual countries (biota monitoring excluded).

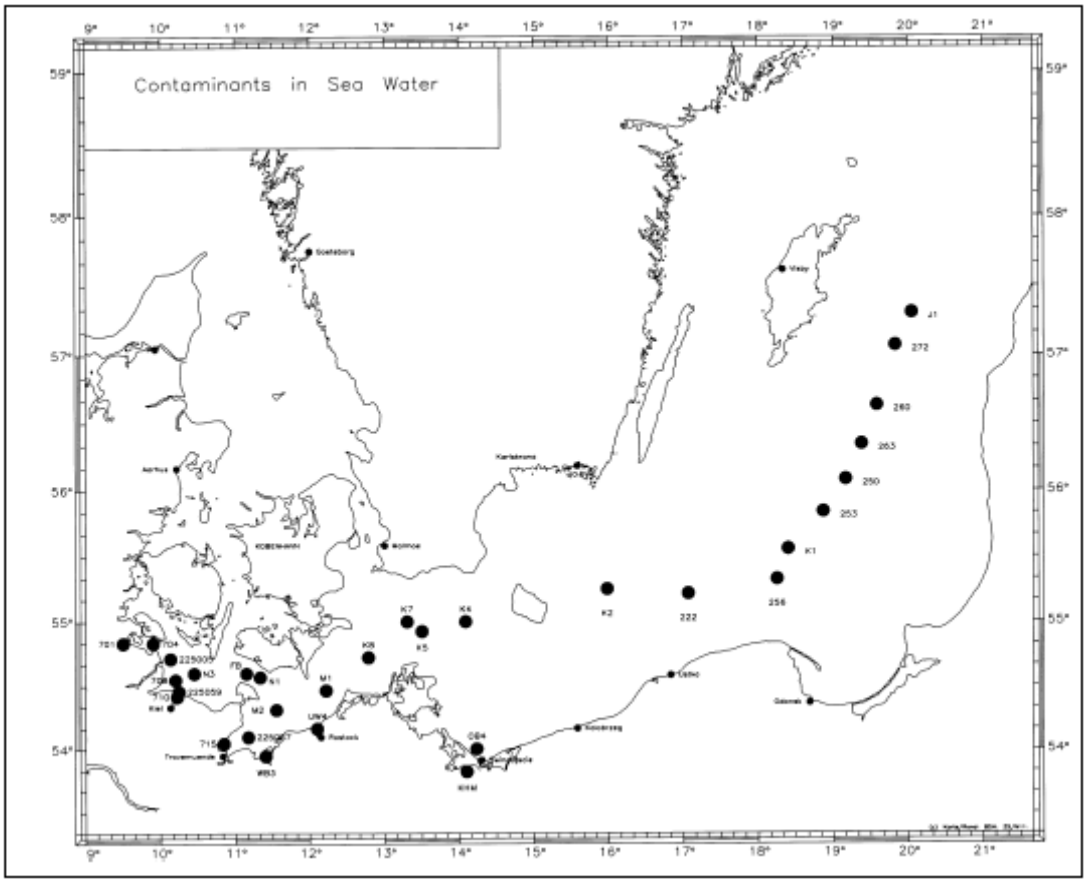


Figure 2 – Baltic sea monitoring within HELCOM. (from http://www.helcom.fi/groups/monas/CombineManual/PartD/en_GB/main/)

Country	***Substances monitored***
Denmark	hexachlorobenzene (HCB), DDT, hexachlorocyclohexane (HCH) (i.a. chlordane, dieldrin), PCBs, PAH and organotin, p-nonylphenols (+ethoxylates), phthalates (DEHP), Linear Alkyl Sulphonates (LAS) (detergents), PAH, pesticides (atrazine, simazine), Tributyltin, Irgarol, brominated flame retardants, tris(4-chlorophenyl)methanol and tris(4-chloro-phenyl)methane, planar CBs, toxaphene.
Estonia	total oil hydrocarbons in sea water (fluorometric analysis)
Finland	total oil hydrocarbons in sea water (fluorometric analysis)
Germany	9 CB congeners, DDTs, HCH, HCB, PAHs (15 compounds) and 30 petroleum hydrocarbons
Latvia	total oil hydrocarbons (fluorometric, determination); 7 stations sampled 4 times per year (February, May, August, November)
Lithuania	Organochlorines - 3 stations;
Poland	In sediment: organic toxicants once in five years from 9 sites

Table 1 – substances monitored by HELCOM Countries.

3. Previous assessments

3.1 EMEP

The MSCE-POP model run at the Meteorological Synthesizing Centre - East of EMEP (http://www.msceast.org/modelling.html) provides estimations of chemical concentrations in air, soil, vegetation, and seawater for selected POPs. At present, the following chemicals are supported: PAHs (B[a]P, B[b]F , B[k]F, I_P), PCB-153, PCDD/Fs, g-HCH, HCB.

3.2 HELCOM reports

The HELCOM has published several reports on pollution loads to the Baltic sea. The latest compilation dates to 20043. These assessments are limited to nutrients and metals, although they provide information on wastewater input and other inputs to the sea waters. A specific report has been issued for dioxins in 20044, quantifying the different emissions to seawater.

[3] HELCOM: The Fourth Baltic Sea Pollution Load Compilation (PLC-4) (2004) http://www.helcom.fi/stc/files/Publications/Proceedings/bsep93.pdf

[4] HELCOM: Dioxins in the Baltic sea, (2004) http://helcom.navigo.fi/stc/files/Publications/OtherPublications/Dioxins_in_BS-2004.pdf

3.3 OSPAR reports

The OSPAR Commission conducts periodical assessment of the loads of chemicals to coastal waters and open sea through the analysis of monitoring data.
The latest OSPAR report on the assessment of monitoring data (2005)5 does not provide any information on organic chemicals, whereas it reports of nutrients and metals.
The Quality Status Report 2000 for the North-East Atlantic6 presents, both for the whole sea area of interest and of individual regional seas, a chapter on chemical pollution (chapter IV), including organic chemicals in the OSPAR list of priority substances. .
In addition, OSPAR publishes a number of background documents on individual chemicals or groups of chemicals in the marine environment, or as a source of contamination for the marine environment. Among others, the following background documents (or other significant documents) are available.

substance	***Publication***
Musk Xylene	2004 No. 200
Trichlorobenzenes	2003 No. 170
Organic Tin Compounds	2000 No. 103
Hexachlorocyclopentadiene (HCCP)	2004 No. 204
POPs from large combustion installations	1997 No. 60
PAHs	2001 No. 137
PCBs	2001 No. 134 (2004 update)
Use of pesticides (II)	1997 No. 70
Paint products, short chain chlorinated paraffines	1996 No. 54
Use of pesticides (I)	1996 No. 55

Table 2 – reports available from OSPAR

3.4 Risk assessment reports

European legislation prior to the entry into force of the REACH regulation required the development of risk assessment reports for individual substances or groups of substances, according to given specifications. At the present time, a number of risk assessment reports have been laid down, either in draft or final form. These reports are now accessible through the JRC web site7, and summarized as follows.

1) Risk assessment reports

Date	**Description**
16-Jan-2006	R2-ethylhexyl acrylate

[5] OSPAR: 2005 Assessment of data collected under the OSPAR Comprehensive Study on Riverine Inputs and Direct Discharges for the period 1990 – 2002
http://www.ospar.org/documents/DBASE/Publications/p00233_RID%20assessment%20report%201990_2002.pdf
[6] OSPAR: Quality Status Report 2000 for the North-East Atlantic – chapter IV
http://www.ospar.org/content/content.asp?menu=00650830000000_000000_000000
[7] http://ecb.jrc.ec.europa.eu/home.php?CONTENU=/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT

Date	Description
20-Nov-2008	2-furaldehyde
19-Nov-2008	2-nitrotoluene
31-Jul-2002	4-nonylphenol and nonylphenol
25-Nov-2004	1,4-dichlorobenzene
28-Nov-2008	2,4-dinitrotoluene
21-Dec-2006	3,4-dichloroaniline
20-Sep-2002	acetonitrile
18-Dec-2003	acrylaldehyde
29-Nov-2002	acrylamide
28-Feb-2003	acrylic acid
07-Apr-2004	Acrylonitrile
14-Nov-2008	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2naph-thyl)ethan-1-one (AHTN)
13-Jan-2005	aniline
13-Feb-2008	benzyl butyl phthalate
08-Oct-2003	4,4'-isopropylidenephenol (bisphenol-A)
29-Jul-2005	but-2-yne-1,4-diol
20-Sep-2002	1,3-butadiene
20-Dec-2007	cadmium metal
20-Dec-2007	cadmium oxide
21-Nov-2008	Chlorodfiluoromethane
19-Nov-2008	(-chloro-2-hydroxypropyl) trimethylammonium chloride (CHPTAC)
30-Jun-2005	chromium trioxide
30-Jun-2005	sodium chromate
30-Jun-2005	sodium dichromate
30-Jun-2005	ammonium dichromate
30-Jun-2005	potassium dichromate
27-Mar-2002	Cumene
12-Feb-2004	Cyclohexane
13-Oct-2003	bis(pentabromophenyl) ether [decabromodiphenyl ether]
07-Feb-2002	2-(2-butoxyethoxy)ethanol
15-Dec-2000	2-(2-methoxyethoxy)ethanol
05-Jun-2008	bis(2-ethylhexyl) phthalate (DEHP)
11-Feb-2004	dibutyl phthalate
07-Aug-2003	1,2-Benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich and: di-"isodecyl" phthalate (DIDP)
31-Jul-2002	dimethyl sulphate
07-Aug-2003	1,2-Benzenedicarboxylic acid, di-C8-10-branched alkyl esters, C9-rich, and: di-"isononyl" phthalate (DINP)
16-Oct-2002	1,4-dioxane, CAS#: 123-91-1
31-Jul-2002	dimethyldioctadecylammonium chloride (dodmac)
03-Jan-2005	edetic acid (EDTA)

Date	Description
31-Jan-2007	2-buthoxyethanol acetate (EGBEA)
01-Feb-2007	2-buthoxyethanol (EGBE)
31-Oct-2008	2,3-epoxypropyltrimthylammonium chloride (EPTAC)
31-Jul-2002	Ethyl acetoacetate
08-Sep-2008	Hexabromocyclododecane
20-Nov-2008	hexachlorocyclopentadiene (HHCP)
27-May-2003	Hydrogen fluoride
12-Nov-2008	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylin-deno[5,6-c]pyran (HHCB)
29-Oct-2003	Hydrogen peroxide
22-Aug-2001	Benzene, C10-13-alkyl derives
30-Mar-2005	monochloroacetic acid (MCAA)
01-Dec-2005	alkanes, C14-17, chloro,
27-May-2002	4,4'-methylenedianiline
16-Jan-2006	methylenediphenyl diisocyanate (mdi)
29-Nov-2002	methacrylic acid
19-Nov-2008	Methenamine
28-Aug-2003	methyl acetate
21-Oct-2002	methyl methacrylate
06-Nov-2002	methyloxirane
20-Sep-2002	tert-buthyl methyl ether
16-Jan-2006	4'-tert-butyl-2',6'-dimethyl-3',5'-dinitroacetophenone (musk ketone)
29-Jul-2005	5-tert-butyl-2,4,6-trinitro-m-xylene (musk xylene)
22-Dec-2003	n-pentane
04-Jan-2005	tetrasodium ethylenediaminetetraacetate (Na4EDTA),
14-Jul-2003	naphthalene
14-Feb-2008	nitrobenzene
23-Dec-2005	trisodium nitrilotriacetate (Na3NTA)
21-Aug-2002	o-anisidine
13-Oct-2003	diphenyl ether, octabromo derivative
31-Jul-2002	4-chloro-o-cresol (pcoc)
27-Apr-2002	diphenyl ether, pentabromo derivative
28-Sep-2007	perboric acid, sodium salt
01-Feb-2007	2-methoxy-1-methylethyl acetate (PGMA)
31-Jan-2007	1-methoxypropan-2-ol (PGME)
21-Dec-2006	phenol
28-Oct-2005	piperazine
26-Aug-2008	propan-1-o
16-Jul-2008	alkanes, C10-13, chloro
20-Dec-2007	sodium hydroxide
17-Dec-2002	styrene
20-Feb-2007	2-methoxy-2-methylbutane (TAME

Date	Description
05-Apr-2006	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol (tetrabromobisphenol-A or TBBP-A)
23-Dec-2005	tetrachloroethylene
29-Jul-2003	toluene
31-Jan-2003	1,2,4-trichlorobenzene
16-Feb-2004	trichloroethylene
04-Dec-2003	1-vinyl-2-pyrrolidone
03-Sep-2004	zinc chloride
13-Oct-2004	zinc distearate
01-Sep-2004	zinc metal
08-Nov-2005	zinc oxide
15-Sep-2004	trizinc bis(ortophosphate)
15-Sep-2004	zinc sulphate

2) Draft risk assessment reports

Date	Description
08-Jul-2002	bis(pentabromophenyl)ether
14-Feb-2002	buta-1,3-diene
05-Feb-2008	n-cyclohexylbenzothiazole-2-sulphenamide (CBS)
18-Jun-2001	di-"isodecyl" phthalate ,
11-Dec-2007	1,2-Benzenedicarboxylic acid, di-C9-11-branched alkyl esters, C10-rich, sodium hypochlorite
29-Aug-2008	chloroform
29-Aug-2008	ethylbenzene
25-Jul-2008	vinyl acetate
13-Feb-2008	4-methyl-m-phenylenediamine (toluene-2,4-diamine)
31-Aug-2005	2-ethoxyethyl acetate
23-Mar-2006	tris(2-chloroethyl) phosphate (TCEP)
14-Dec-2005	2,4,4-trimethylpentene
05-Feb-2008	zinc phosphate
10-Dec-2007	bis(hydroxylammonium)sulfate
31-Mar-2006	nickel
31-Mar-2006	nickel sulphate
13-Feb-2002	tert-butyl methyl ether
10-Aug-2005	anthracene
06-Feb-2008	chlorine
03-May-2004	tert-butyl hydroperoxide (TBHP)
14-Jul-2003	musk ketone
14-Jul-2003	musk xylene
11-Dec-2007	coal tar pitch, high temperature (CTP(ht))
25-Mar-2003	chromium trioxide

Date	Description
01-Sep-2008	4-tert-butylphenol
14-Sep-2007	4-tert-butylbenzoic acid
31-Mar-2006	nickel carbonate
31-Mar-2006	nickel chloride
31-Mar-2006	nickel dinitrate,
23-Mar-2006	Tris(nonylphenyl) phosphite (TNPP)

Risk assessment reports may be useful in the assessment of loads of hazardous substances, as they provide a wealth of information on substances including emissions and fate. However, the information is not in spatially distributed form and only allows a general overall assessment.

3.5 Pesticides

Pesticides are the subject of specific analysis in the last years. In particular, they are the topic of an agri-environmental indicator in the IRENA indicator system8. However, at present the only source of information at European scale is the report issued by EUROSTAT on aggregated consumption of pesticides from the ECPA member companies, accounting for about 90% of the market value (but, likely, less in terms of mass)9. These pesticide use data provide figures for broad chemical substance classes, for the whole European Union (excluding Bulgaria and Romania, which were not members at the time of reporting), grouped by crop class. A number of assessment exercises have been conducted for Europe based on different types of models. These are briefly reviewed elsewhere10. However, at present there is no single entry point for the collection and analysis of pesticides in Europe.

3.6 Eurochlor assessments

The European Chlorine chemical industry association has issued a number of marine risk assessment reports. Substances covered by the assessment are:1,2-dichloroethane,, 1,1,1-trichloroethane, 1,1,2-trichloroethane, Vinyl, chloride, Tetrachloroethylene, Monochlorobenzene, Trichloroethylene, 1,2-dichlorobenzene, Chloroform, 1,4-dichlorobenzene, Monochloromethane, Carbon, tetrachloride, Mercury, Dichloromethane, Monochlorophenols, (2-,, 3-, and, 4-monochlorophenol),

[8] For example, EEA – Agriculture and Environment in EU15 – the IRENA indicator report, EEA Report N 6/2005. Indicator fact sheets are available from http://eea.eionet.europa.eu/Public/irc/eionet-circle/irena/library?l=/final_delivery/indicator_sheets&vm=detailed&sb=Title ; data sheets are available from http://eea.eionet.europa.eu/Public/irc/eionet-circle/irena/library?l=/final_delivery/data_sheets&vm=detailed&sb=Title

[9] EUROSTAT, The use of plant protection products in the European Union (2007 Edition), Data 1992-2003. ISBN 92-79-03890-7. Luxembourg: Office for Official Publications of the European Communities, 2007

[10] Pistocchi, A., Bidoglio, G., Is it presently possible to assess the spatial distribution of agricultural pesticides for continental Europe? A screening study based on available data. Submitted, 2010.

Hexachlorobenzene, PCBs,, DDT, and, dioxin, Hexachlorobutadiene, Pentachlorophenol, 1,2,4-Trichlorobenzene, 1,1-Dichloroethene.
The reports can be accessed from the Eurochlor web site: http://www.eurochlor.org/index.asp?page=88.

3.7 OECD assessments

OECD reports assessments for individual chemicals or groups of chemicals. In general, although a useful source of information and tools for coordination of chemical management, OECD does not provide systematically original assessment. The reports do not have a serial character. Examples of such reports are the ones on surveys about PFOS11.

3.8 UNEP Chemicals assessments

UNEP, similarly to OECD, coordinates knowledge, data and methods for chemical management. It has published, among other documents, a series of regionally based reports on persistent and toxic substances. Among them, two reports are of interest to Europe: Regionally Based Assessment of Persistent Toxic Substances: Europe Regional Report, and Regionally Based Assessment of Persistent Toxic Substances:Mediterranean Regional Report12. Both reports date back to 2002 and cover atrazine, PBDEs, lindane, organic mercury, organic tin, PCP, PAHs, SCCP, Hexabomobiphenyl, phtalates, nonylphenols, tert-octylphenol, besides the "dirty dozen" Stockholm convention chemicals.

3.9 Selected European projects

A number of European projects have been launched in recent years to address, either as primary or secondary focus, the issue of spatial assessment of hazardous chemicals. The following table provides a quick overview of some selected projects, aiming more at providing examples than at a comprehensive review.

Name	Web site	Topics	Available reports/data
Aquaterra	http://www.attempto-projects.de	River basin management to cope with climate change, land uses and pollution	
Risk base	http://www.riskbase.info	Summarize and synthesize existing projects on risk assessment	
Alarm	http://www.alarmproject.net	Biodiversity and climate cange/pollution	
SOCOPSE	http://www.socopse.se/	Identify viable reduction measures for WFD priority	Atrazine Cadmium Isoproturon

[11] http://www.oecd.org/document/58/0,3343,en_2649_34375_2384378_1_1_1_37465,00.html

[12] The two documents can be accessed online:
http://portalserver.unepchemicals.ch/Publications/RBAPTSEuropeRR.pdf ;
http://portalserver.unepchemicals.ch/Publications/RBAPTSMediterranRR.pdf

Name	Web site	Topics	Available reports/data
		substances; material flow analysis	Mercury PBDE TBT PAH Nonylphenols HCB DEHP
HEIMTSA	http://www.heimtsa.eu	Methods for risk assessment;	case studies
Nomiracle	http://nomiracle.jrc.ec.europa.eu	Methods for risk assessment;	case studies
FOOTPRINT	http://www.eu-footprint.org/	Pesticide risk in water ecosystems	Models and databases
HAIR	http://www.rivm.nl/rvs/overige/risbeoor/Modellen/HAIR.jsp	Pesticide risk indicators	Models and databases

Table 3 – examples of European projects yielding potentially useful information on the spatial modeling of chemicals.

4. Existing emission databases

At present, a number of emission estimates have been developed for POPs. For instance, Breivik et al., 200413, quote existing emission estimates for DDT, HCB, HCHs, PAHs, PCBs, PCDD/Fs, and other POPs. Their summarizing Table 1 is reproduced in Figure 3 for comfort of reading.
Some of these estimates are considered by EMEP that provides emission values, both officially reported and estimated by experts, for selected POPs (HCH, HCB, PCDD/Fs, PCBs, PAHs) among other chemicals. The EMEP emission estimates are provided in gridded form from the web site:
http://www.emep-emissions.at/emission-data-webdab/emissions-used-in-emep-models/

For a number of industrial chemicals, emissions to air and water from industrial facilities falling under the IPPC regulations are provided through the EPER database, which is accessible from the web site: http://eper.ec.europa.eu/ . These emissions seem to provide quite high standards of quality and certainty with comparison to emission estimates (which are usually considered certain within at least +/- one order of magnitude. On the other hand, they only account for large industrial plant emissions at the European scale,

[13] Knut Breivik, Ruth Alcock, Yi-Fan Li, Robert E. Bailey, Heidelore Fiedler, Jozef M. Pacyna, Primary sources of selected POPs: regional and global scale emission inventories, Environmental Pollution, Volume 128, Issues 1-2, Persistant Organic Pollutants, March 2004, Pages 3-16, ISSN 0269-7491, DOI: 10.1016/j.envpol.2003.08.031. (http://www.sciencedirect.com/science/article/B6VB5-49Y9BS4-D/2/8a45fa594510eb77178a8b0ad2bfe914)

which might reflect some 10 % or less of total emission for some chemicals[14]. To broaden the scope of EPER, both in terms of substances considered and sources of emission, a new E-PRTR regulation has been adopted which is expected to lead to new reports on emissions by 2009. A pilot emission inventory has been published at the site: http://www.bipro.de/__prtr/index.htm. The pollutants covered by EPER are provided in the following table, along with the emission thresholds for reporting by industrial facility.

Substance	Thresholds to air (per year)	Thresholds water (per year)
Ammonia, NH3	10.00 t	-
Arsenic and its compounds	0.02 t	0.01 t
Benzene	1.00 t	-
Benzene, toluene, ethylbenzene, xylenes (as BTEX)	-	0.20 t
Brominated diphenylethers	-	0.00 t
Cadmium and its compounds	0.01 t	0.01 t
Carbon dioxide, CO2	100,000.00 t	-
Carbon monoxide, CO	500.00 t	-
Chlorides	-	2,000.00 t
Chlorine and inorganic compounds (as HCl)	10.00 t	-
Chloro-alkanes (C10-13)	-	0.002 kg
Chromium and its compounds	0.10 t	0.05 t
Copper and its compounds	0.10 t	0.05 t
Cyanides, total CN	-	0.05 t
Dichloroethane-1,2 (DCE)	1.00 t	0.01 t
Dichloromethane (DCM)	1.00 t	0.01 t
Dioxins and furans (PCDDs and PCDFs)	0.001 kg	-
Fluorides	-	2.00 t
Fluorine and inorganic compounds (as hydrogen fluoride)	5.00 t	-
Halogenated Organic Compounds (AOX)	-	1.00 t
Hexachlorobenzene (HCB)	0.01 t	0.00 t
Hexachlorobutadiene (HCBD)	-	0.00 t
Hexachlorocyclohexane (HCH)	0.01 t	0.00 t
Hydrofluorocarbons (HFCs)	0.10 t	-
Hydrogen cyanide (HCN)	0.20 t	-
Lead and its compounds	0.20 t	0.02 t
Mercury and its compounds	0.01 t	0.00 t
Methane, CH4	100.00 t	-
Nickel and its compounds	0.05 t	0.02 t
Nitrogen oxides, NOx	100.00 t	-
Nitrogen, total	-	50.00 t
Nitrous oxide (N2O)	10.00 t	-
Non methane volatile organic compounds	100.00 t	-

[14] See figures provided in the section "Questions to EPER" of the EPER web site: http://eper.ec.europa.eu/eper/faq.asp?i= , question #5.

Substance	Thresholds to air (per year)	Thresholds water (per year)
(NMVOC)		
Organotin compounds	-	0.05 t
Pentachlorophenol (PCP)	0.01 t	-
Perfluorocarbons (PFCs)	0.10 t	-
Phenols	-	0.02 t
Phosphorus, total	-	5.00 t
PM10 (Particulate matter less than 10 µm)	50.00 t	-
Polycyclic Aromatic Hydrocarbons (PAH)	0.05 t	0.01 t
Sulphur hexafluoride (SF6)	0.05 t	-
Sulphur oxides (SOx)	150.00 t	-
Tetrachloroethylene (PER)	2.00 t	-
Tetrachloromethane (TCM)	0.10 t	-
Total Organic Carbon (TOC)	-	50.00 t
Trichlorobenzenes (TCBs)	0.01 t	-
Trichloroethane-1,1,1 (TCE)	0.10 t	-
Trichloroethylene (TRI)	2.00 t	-
Trichloromethane (Chloroform)	0.50 t	-
Zinc and its compounds		

Table 4 – EPER chemicals

The prospective 91 E-PRTR chemicals are:

1. Methane (CH4)
2. Carbon monoxide (CO)
3. Carbon dioxide (CO2)
4. Hydro-fluorocarbons (HFCs)
5. Nitrous oxide (N2O)
6. Ammonia (NH3)
7. Non-methane volatile organic compounds (NMVOC)
8. Nitrogen oxides (NOx / NO2)
9. Perfluorocarbons (PFCs)
10. Sulphur hexafluoride (SF6)
11. Sulphur oxides (SOx / SO2)
12. Total nitrogen
13. Total phosphorus
14. Hydrochlorofluorocarbons (HCFCs)
15. Chlorofluorocarbons (CFCs)
16. Halons
17. Arsenic and compounds (as As)
18. Cadmium and compounds (as Cd)
19. Chromium and compounds (as Cr)
20. Copper and compounds (as Cu)
21. Mercury and compounds (as Hg)
22. Nickel and compounds (as Ni)
23. Lead and compounds (as Pb)
24. Zinc and compounds (as Zn)
25. Alachlor
26. Aldrin
27. Atrazine
28. Chlordane
29. Chlordecone
30. Chlorfenvinphos
31. Chloro-alkanes, C10-C13
32. Chlorpyrifos
33. DDT
34. 1,2-dichloroethane (EDC)
35. Dichloromethane (DCM)
36. Dieldrin
37. Diuron
38. Endosulphan
39. Endrin
40. Halogenated organic compounds (as AOX)
41. Heptachlor
42. Hexachlorobenzene (HCB)
43. Hexachlorobutadiene (HCBD)
44. 1,2,3,4,5,6-hexachlorocyclohexane(HCH)
45. Lindane

46. Mirex
47. PCDD +PCDF (dioxins + furans) (as Teq)
48. Pentachlorobenzene
49. Pentachlorophenol (PCP)
50. Polychlorinated biphenyls (PCBs)
51. Simazine
52. Tetrachloroethylene (PER)
53. Tetrachloromethane (TCM)
54. Trichlorobenzenes (TCBs)
55. 1,1,1-trichloroethane
56. 1,1,2,2-tetrachloroethane
57. Trichloroethylene
58. Trichloromethane
59. Toxaphene
60. Vinyl chloride
61. Anthracene
62. Benzene
63. Brominated diphenylethers (PBDE)
64. Nonylphenol ethoxylates (NP/NPEs) and related substances
65. Ethyl benzene
66. Ethylene oxide
67. Isoproturon
68. Naphthalene
69. Organotin compounds (as total Sn)
70. Di-(2-ethyl hexyl) phthalate (DEHP)
71. Phenols (as total C)
72. Polycyclic aromatic hydrocarbons (PAHs)
73. Toluene
74. Tributyltin and compounds
75. Triphenyltin and compounds
76. Total organic carbon (TOC) (as total C or COD/3)
77. Trifluralin
78. Xylenes
79. Chlorides (as total Cl)
80. Chlorine and inorganic compounds (as HCl)
81. Asbestos
82. Cyanides (as total CN)
83. Fluorides (as total F)
84. Fluorine and inorganic compounds (as HF)
85. Hydrogen cyanide (HCN)
86. Particulate matter (PM10)
87. Octylphenols and Octylphenol ethoxylates
88. Fluoranthene
89. Isodrin
90. Hexabromobiphenyl
91. Benzo(g,h,i)perylene.

Out of these chemicals, only 23 substances or groups of substances are presently included in the pilot implementation, and only for emissions to air. The source of information is usually the EMEP emission inventory, except for greenhouse gases. The 23 substances are: Methane (CH4), Carbon monoxide (CO), Carbon dioxide (CO2), Nitrous oxide (N2O), Ammonia (NH3), Non-methane volatile organic compounds (NMVOC), Nitrogen oxides (NOx/NO2), Sulphur oxides (SOx/SO2), Arsenic and compounds (as As), Cadmium and compounds (as Cd), Chromium and compounds (as Cr), Copper and compounds (as Cu), Mercury and compounds (as Hg), Nickel and compounds (as Ni), Lead and compounds (as Pb), Zinc and compounds (as Zn), Hexachlorobenzene (HCB), 1,2,3,4,5,6-hexachlorocyclohexane(HCH), PCDD +PCDF (dioxins +furans) (as Teq), Pentachlorophenol (PCP), Polychlorinated biphenyls (PCBs), Polycyclic aromatic hydrocarbons (PAHs), Particulate matter (PM10). For emissions to water, only nutrient emissions are presently implemented in the pilot database. No emission to land is implemented. The sectors of emission so far identified include:

- for air:
  - Road transport
  - Shipping
  - Aviation
  - Railway
  - Military
  - Domestic fuel combustion
  - Solvent use
  - Fossil fuel distribution

- Roofing and road paving with asphalt
- Agriculture

- for water:
  - Total diffuse Natural background losses
  - Agriculture
  - Scattered dwellings
  - Anthropogenic diffuse sources.

Table 1
Selected emission inventories for POPs with regional and global scale coverage

Chemical(s)							Mode of release	Spatial characteristics		Temporal characteristics		Notes	Reference(s)
DDT	HCB	HCHs	PAHs	PCBs	PCDD/Fs	Other		Coverage	Distribution	Coverage	Distribution		
	X						Atmospheric	Global	–	~1995	Annual		Bailey, (2001a)
	X	X	X	X	X	[1]	Atmospheric	Europe	By Country	1990	Annual	[A]	Berdowski et al. (1997)
		X					Total	Europe	By Country	1990–1996	Annual		Breivik et al. (1999)
				X			Atmospheric	Global	By Country	1930–2000	Annual		Breivik et al. (2002a,b)
					X		Land, Water	Europe	By Country	~1994	Annual	[B]	Buckley-Golder et al. (1999)
					X		Land	Global	By Country	~2000			Dyke (2003)
					X		Atmospheric	Global	By Country	~2000	Annual		Fiedler (2003)
		X					Atmospheric	Global	1x1 lat/long	1948–2000	Annual		Li et al. (2000, 2003)
						[2]	Atmospheric	USA	1/4x1/6 lat/long	1947–2000	Annual		Li et al. (2001b)
X							Atmsopheric	Global	1x1 lat/long	1945–2000	Annual		Li (2003a)
X							Atmospheric	USA	1/4x1/6 lat/long	1945–2000	Annual		Li (2003b)
				X			Total	N. America	–	1930–1970	Historical		Nisbet amd Sarofim (1972)
					X		Atmospheric (Mainly)	Global	By Country	1995	Annual		UNEP (1999)
X	X	X	X	X	X	[3]	Atmospheric	Europe/USA	By Country	1980–2000	Annual	[C]	Vestreng and Klein (2002)
X	X		X		X		Atmospheric	Europe	By Country	1970–1995	Each 5th year	[A]	Pacyna et al. (2003)
					X		Multimedia	Europe	By Country	~1994	Annual	[B]	Quass and Fermann (1997)

[1] Endosulfan, Fenthione, Quintizene, Pentachlorophenol, Tetrachloroethene, Trichloroethene, Trichlorobenzene, 1,1,1-Trichloroethane, Tetrachloromethane, Xylene. [2] Toxaphene. [3] Aldrin, Chlordane, Chlordecone, Dieldrin, Endrin, Heptachlor, Hexabromobiphenyl, Mirex, Toxaphene, PCP, SCCP, PER, TRI. [A] The data are a mixture of official data submitted by the countries and default project estimates. [B] Fifteen EU countries plus Norway and Switzerland. [C] Official data submitted to UNECE/EMEP by 31 different countries. The data generally have a limited spatial/temporal and compound coverage.

Figure 3 – snapshot of Table 1 in Breivik et al., 2004

5. Summary of model options and strategies for the analysis of scenarios

There are a very high number of hazardous substances (HS) that warrant characterizing their spatial distribution in the environment, and particularly their loads to coastal regions. Policy contexts requiring an assessment of HS include international agreements (Aarhus Protocol and Stockholm Convention), the WFD and Marine Directive, pesticide management, industrial pollution management, and the management of chemicals in general. Despite the abundance of policies calling for assessment, so far the available knowledge, and predictive capability, concerning HS is rather limited.
The required knowledge about HS in order to assess their present and predicted future spatial distribution can be classified in:

- physico-chemical properties
- emissions to the different environmental compartments
- factors affecting environmental fate and transport
- monitored concentrations in the environment.

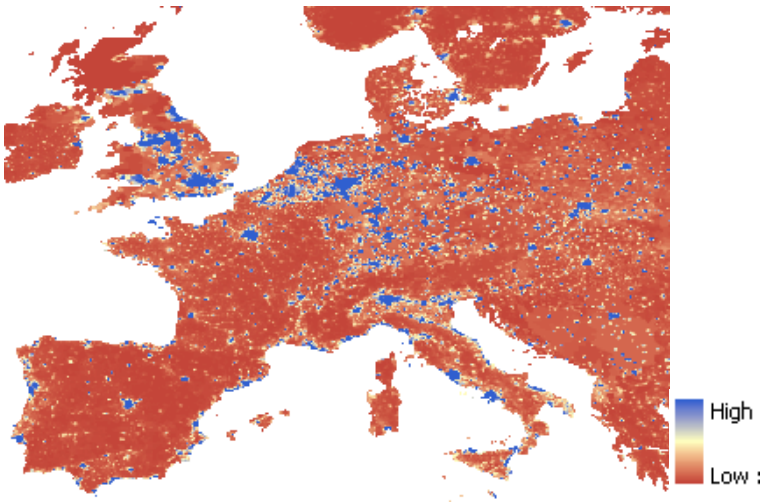
Physico-chemical properties of substances are generally quite well known or easy to determine. Nevertheless, some properties easily measurable in the laboratory do not reflect the actual behavior of substances in the environment. This is particularly true for degradation, which is affected by a number of factors difficult to accurately and completely reproduce in laboratory conditions. As a first approximation, however, physico-chemical properties may be considered known for all chemicals of concern.

Emissions are maybe the most difficult knowledge component for HS. The risk assessment reports and other specific studies may sometimes support in the estimation of the overall quantity of a given chemical used or emitted over one region or the world, through mass balances and similar calculations. However, for fate and transport assessment it is often essential to know also the spatial distribution of emissions beside absolute quantities. This implies the modeling of emission patterns using supporting spatial distributions of potential emitters. Typical such support patterns include population density, or equivalently the distribution of intensity of lights at night[15], or indicators of agriculture and other land uses. Lights at night, in particular, indicate generic human activity and may represent a suitable spatial distribution for all emissions related to widespread use of chemicals (see Figure 4). The distribution of lights at night is similar, but not fully coincident, with the distribution of population (see Figure 5). The latter, in particular, is usually available with the resolution of municipality boundary polygons. Moreover, it does not reflect other chemical-emitting human activities (e.g. large industrial complexes) outside of highly populated areas.

[15] See the description of the approach in Christopher D. Elvidge, Marc L. Imhoff, Kimberly E. Baugh,Vinita Ruth Hobson, Ingrid Nelson, Jeff Safran, John B. Dietz, Benjamin T. Tuttle, Night-time lights of the world: 1994–1995 ISPRS Journal of Photogrammetry & Remote Sensing 56 (2001) 81– 99. Data can be downloaded from http://www.ngdc.noaa.gov/dmsp/global_composites_v2.html

Agriculture and other land-use related patterns can be quantified for the European region through the data of the Corine Land Cover 2000 map. For instance, Pistocchi et al., 200816 use patterns of intensity of different agricultural land uses to build emission maps for pesticides (Figure 6).

Figure 4– example of the distribution of lights at night in Europe and the Mediterranean region.



16 Pistocchi, A., Vizcaino, P., Hauck, M., A GIS model-based screening of potential contamination of soil and water by pyrethroids in Europe, Journal of Environmental Management, Volume 90, Issue 11, August 2009, Pages 3410-3421

Figure 5– example of the distribution of population, from the Gridded Population of the World - GPW 3.0 product[17].

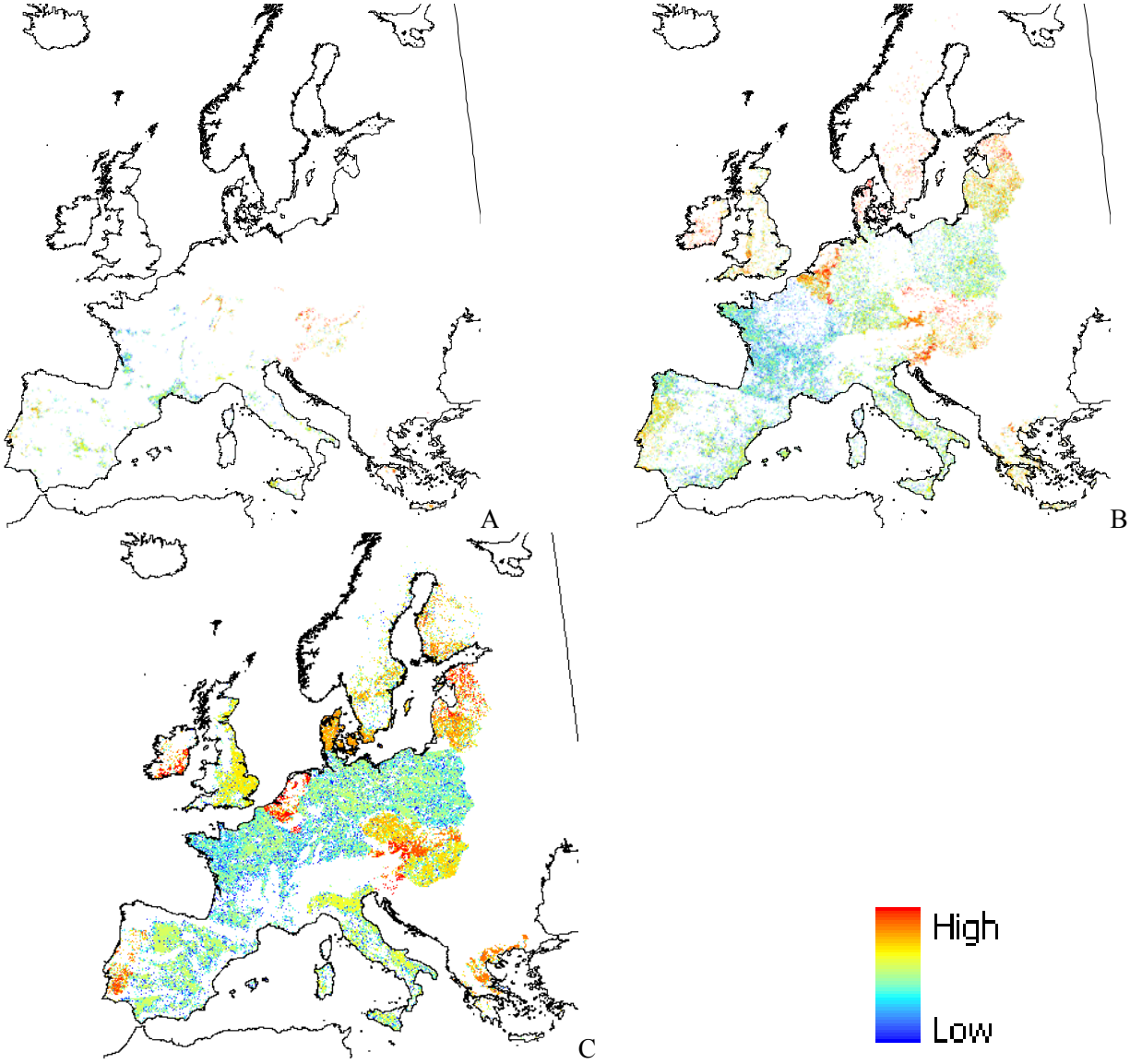


Figure 6 - spatial distribution of vine/grape intensity (A), arable crop intensity (B), permanent crop intensity (C), from CORINE Land Cover 2000.

In some cases, emissions are already estimated in gridded data. This is the case of EMEP grids of emission, or other emission inventories.
For the European industrial emission inventory EPER, data are precisely georeferenced and come as points in space (Figure 7). In this case, emissions can be used directly for the quantification of the spatial distribution of chemicals.

[17]Documentation and data available at http://sedac.ciesin.columbia.edu/gpw/

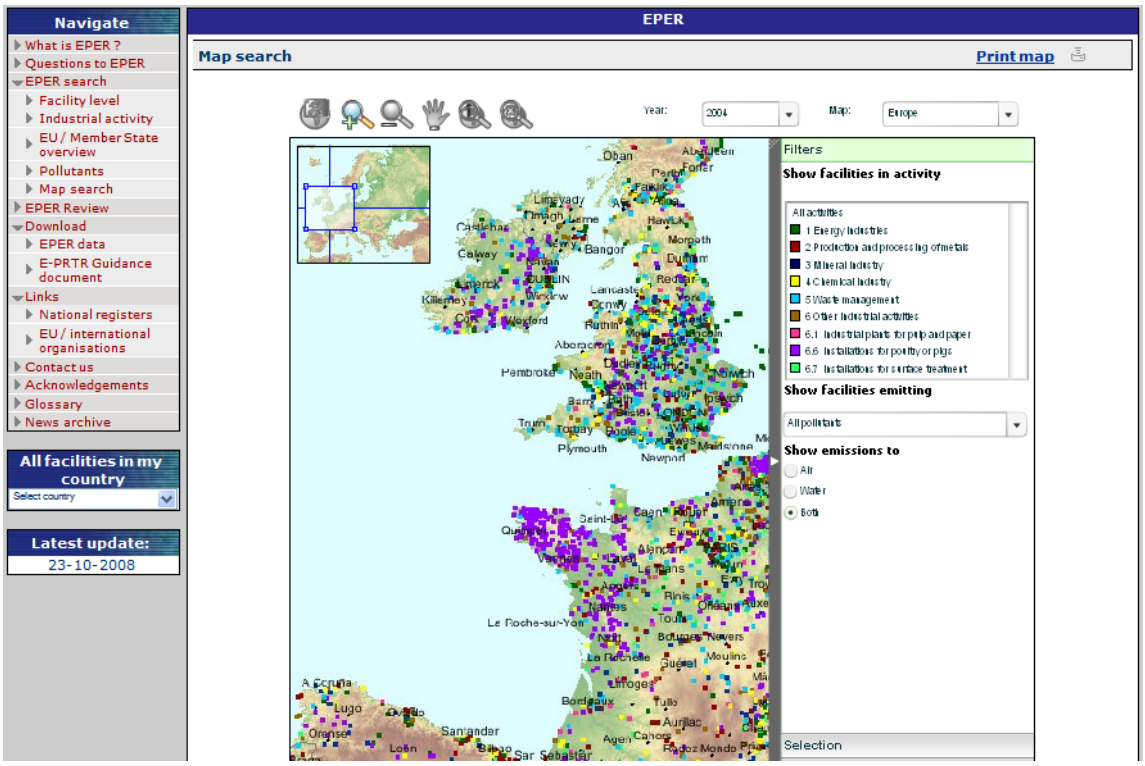


Figure 7 – distribution of emission points in EPER: example of the web-GIS interface[18]

Relevant landscape and climate parameters for fate and transport of chemicals include weather, soil properties, vegetation, hydrology, atmospheric transport patterns, and similar attributes. An extensive discussion of variables usually adopted to describe fate and transport of chemicals, and the data sets available for their representation, is presented in Pistocchi et al., 200619. It can be said that, at present, landscape and climate data for model parameterization is not the main issue. Rather, models still lack well established algorithms for the specific representation of physical processes20.

Monitored concentrations in the environment are key to any model application. Although considerable effort has been spent in many national and international projects, at present monitoring datasets for many of the HS of concern are still lacking. The usual practice is to search the literature, on a case-by-case basis, to retrieve data whenever needed for model evaluation. This produces a high dispersion of efforts and prevents the building of consistent, quality-checked databases. Although in the future the policy context is promising to fill this gap by forcing the different actors to collect and share data,

[18] http://eper.eea.europa.eu/eper/flashmap.asp

[19] Pistocchi, A., Vizcaino, M.P., Pennington, D.W. (2006). Analysis of Landscape and Climate Parameters for Continental Scale Assessment of the Fate of Pollutants . EUR 22624 EN ISSN: 1018-5593 ISBN: 978-92-79-04809-8. Luxembourg: Office for Official Publications of the European Communities. http://fate.jrc.ec.europa.eu/mappe/data/doc/ALPaCA.pdf

[20] See discussion in Nomiracle IP D2.4.6 Pistocchi, A., Report on an optimised multimedia fate and human exposure model with various spatial resolutions at the European level. http://nomiracle.jrc.it/Documents/PublicDeliverables/D.2.4.6%20Report%20on%20an%20optimised%20multimedia%20fate%20and%20human%20exposure%20model.pdf

presently there is a need to capitalize on published literature, including "grey literature" and easily accessible web sites where national or regional authorities in Europe make their data available.

From the overview presented above, we can state that any scenario study of individual HS in Europe requires extensive collection of information, including physico-chemical properties, modes of use of the substance, statistics of absolute quantities used and emitted, and monitored concentrations in the environment. Based on this information, there is usually a need to develop a spatial model of emission, typically through the use of emission patterns as discussed above. Once emission estimates are available, a model can be run to predict environmental concentrations to be compared with monitoring data. Although models of very sophisticated detail have been developed, at present it seems preferable to use simple GIS-based approaches to predict the spatial distribution of HS[21] and, consequently, loads to the coastal waters. Given the uncertainty in both emission distribution, and (most of the times) the precise physics of chemical fate in the environment, it is very difficult to go beyond an accuracy of one order of magnitude in the prediction of environmental concentrations. Also, experience shows that the attainable correlation of observations and predictions usually corresponds to not more than 50% explained variance, irrespective of the detail level of the model, although examples do exist of case studies (usually referred to a limited region in space) where higher accuracy is obtained, at the cost of much higher data gathering and model development as well as computational burden.

The number of priority HS in Europe is of the order of 1000 chemicals, i.e. 1% of the chemicals used in Europe; however, the potential relevance of a substance may largely depend on site specific issues such as use patterns, climate and ecosystem distribution etc. This is particularly true for hazardous but volatile and/or short-lived compounds, or, on the other extreme, slow-moving or immobile compounds such as those adsorbing to solids in soils and sediments.

In chapter 7 we will focus on 3 example chemicals, which will be studied to the maximum possible extent at continental scale, given the present model capability and level of knowledge. However, a general challenge for the overall study of HS is to describe virtually all substances of concern, so that cumulative effects can be also tackled. As emissions are almost necessarily an estimate, and their modeling implies use of a relatively limited number of spatial patterns (population density, agriculture, etc.), it is not unrealistic to think of setting up a modeling framework capable to represent emissions for virtually all chemicals using standardized emission patterns as a first approximation. In this respect, the three substances to e selected are to be seen as an example for future generalized studies.

It is worth mentioning that, generally speaking, scenario studies need to cope not only with trends in the use of chemicals in response to policy implementation, but also in issues such as climate change, socioeconomic variations etc. Modeling scenarios is a very complex task. However, for the specific case of HS, scenarios may be studied as a first approximation as one of the following options:

- "business as usual" and chemical use extrapolated from current trend

[21] Pistocchi, A. (2008). A GIS-based approach for modeling the fate and transport of pollutants in Europe, Environmental Science and Technology, 42, 3640-3647.

- Restrictions to the use of the chemical
- Ban of the chemical within a given time frame.

The first option corresponds to chemicals not yet regulated. The use of such chemicals is controlled only by market, technology and consumer preferences. Only a detailed technical study may reveal these dynamics, whereas the observed used trend over recent years may indicate expanding, shrinking or stationary use of the chemical. Given uncertainties involved in the fate and transport model, it does not seem appropriate to go beyond these simple considerations.

The second option refers to chemicals for which use is not forbidden in general, but it is restricted to certain applications. This may change substantially the mode of entry of the chemical in the environment (e.g. restriction to open air application of a pesticide may leave it as a potential soil pollutant due to seed treatment), beside of course the absolute quantities in use.

The third option refers to the ban of a chemical. Usually the ban is not abrupt but warrants a time frame for the withdrawal of a chemical from use. A simple but reasonable way to simulate this phenomenon is to represent emissions as an exponential decay with DT90 (the time for the emissions to decrease of 90%) given by the timeframe for the ban, T. therefore, emissions at time t are described as:

$$E(t) = E_0 e^{-\frac{\ln(\frac{10}{9})}{T}t}$$

where E0 is present day emission. This corresponds to a fast-reacting market. In other cases, when a chemical which has been banned is difficult or expensive to be replaced, a more appropriate “slow reaction” model should be used, like e.g. a “breakthrough curve” model (Figure 8).

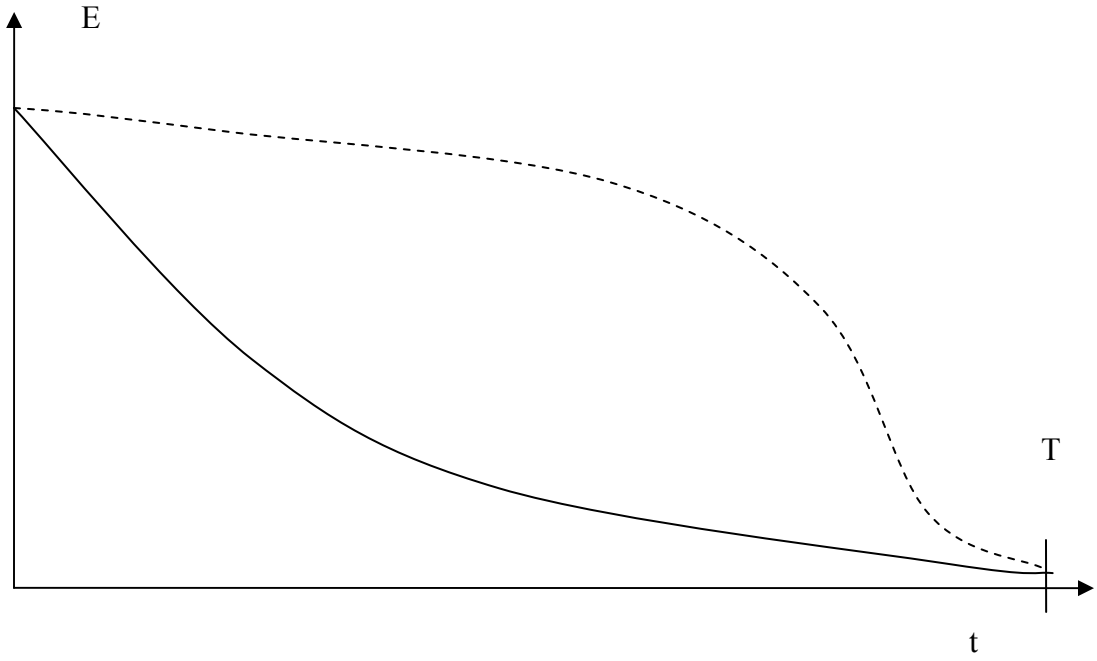


Figure 8 – modes of emission reduction within a ban time frame T.

6. Prioritization and selection of the target chemicals for the present study

Based on the above considerations on the availability of information and open issues in the modeling of priority substances, we layed out a synthetic overview of substances of potential interest in order to develop a detailed analysis in the coming phases of the project.
For what concerns legislation and concern in different policy contexts, the following Table 5 summarizes the situation.

For what concerns the availability of information on the substances, including monitoring, previous studies, emission inventories and the status for ban, the following Table 6 provides an overview. We deliberately excluded metals as our present focus is on organic contaminants.
We did a qualitative check on the level of concern around each chemical, and the availability of data. Based on this preliminary check, we come to the conclusion that the best candidates could be Lindane, PAHs and either endosulfan or trifluralin. In addition, we considered to study PFOS (Perfluorooctansulfonate), which is of high and emerging concern both for inland and marine waters (OSPAR). The latter would have the advantage of being a "new, emerging issue" (for lindane and especially PAHs extensive studies have been carried out by EMEP), but the disadvantage that it might be difficult to

build significant scenarios as history of consumption and phasing out perspectives might be unclear. The JRC has a reasonable pan-European monitoring dataset on PFOS and we could build on this for the analysis.
Endosulphan and trifluralin usage as agricultural pesticides is changing, likely to give a big difference in their source strength in future. PFOS is receiving increasing attention. Lindane may be more a historic substance, with not so much change to model in the future. PAHs are still an issue. An optimum choice seems to need to balance 'some old' (lots of data, but little knowledge to add) with 'some new' (less data, but potentially more to learn).
Based on the above considerations, we selected the following chemicals:
1) Lindane: “old” substance, but useful as a benchmark for modeling – quite some data, still a concern although not so likely to change in scenario conditions
2) Trifluralin: this is maybe the best example substance with respect to the policy context, also in view of the planned outphasing. Use of Endosulfan in Europe seems less widespread: in 2003, 6182 tonnes dinitroaniline herbicides (8 chemicals including trifluralin, the others being far less “POPs”) were reported in use in EU, vs 198 tonnes organochlorine insecticides (4 chemicals: Dicofol, Endosulfan, Lindane, Tetradifon), according to the latest EUROSTAT reports.
3) PFOS: this is a good example of emerging pollutant, while PAHs are already a subject of investigation in other research programmes.

Table 5 - regulations

Substance Name	***Aarhus (CLRTAP)***	***HELCOM rec.19/5 (appendix 3)***	***OSPAR chemicals of priority action (2007 update)***	***WFD***	***Dir. 76/464 Pertinent daughter directive or amendment of 76/769/EEC***	***Stockholm convention (R=regulated; C=candidate)***
Alachlor				X		
Anthracene				X		
Atrazine				X		
Benzene				X		
Brominated diphenylethers		X	X	X		C (pentabromodiphenyl+ octabromodiphenyl ether)
Short chained chlorinated paraffins (SCCP)		X	X	X (as C_{10-13}-chloroalkane)		C
Chlorfenvinphos				X		
Chlorpyrifos				X		
1,2-Dichloroethane		X		X	Dir. 90/415	
Dichloromethane				X		
Di(2-ethylhexyl)phthalate (DEHP)		X	X	X		
Diuron				X		
Endosulfan			X	X		C
Fluoranthene				X		
Hexachlorobenzene	X	X		X	Dir. 88/347	R
Hexachlorobutadiene				X	Dir. 88/347	
Hexachlorocyclohexane	X	X	X	X	Dir. 84/491	C (lindane)
Isoproturon				X		
Naphthalene			X (various naphtalenes)	X		

Table 5 - regulations

Substance Name	***Aarhus*** ***(CLRTAP)***	***HELCOM rec.19/5 (appendix 3)***	***OSPAR*** ***chemicals of priority action (2007 update)***	***WFD***	***Dir. 76/464*** ***Pertinent daughter directive or amendment of 76/769/EEC***	***Stockholm convention (R=regulated; C=candidate)***
Nonylphenols		X (as nonylphenol-4 and nonylphenolethoxylate)	X (as nonylphenol ethoxylate)	X		
Octylphenols			X	X		
Pentachlorobenzene				X		C
Pentachlorophenol		X	X	X	Dir. 86/280	
Polyaromatic hydrocarbons	X	X	X	X		
(Benzo(a)pyrene),	X	X	X	X		
(Benzo(b)fluoranthene),	X	X	X	X		
(Benzo(g,h,i)perylene),		X	X	X		
(Benzo(k)fluoranthene),	X	X	X	X		
(Indeno(1,2,3-cd)pyrene)	X	X	X	X		
Simazine				X		
Tributyltin compounds			X (organic tin compounds)	X		
Trichlorobenzenes			X	X	Dir. 90/415	
Trichloromethane (Chloroform)		X		X	Dir. 88/347	
Trifluralin			X	X		
DDT	X	X		X	Dir. 86/280	R
Aldrin	X	X		X	Dir. 88/347	R
Dieldrin	X	X		X	Dir. 88/347	R

Table 5 - regulations

Substance Name	***Aarhus*** ***(CLRTAP)***	***HELCOM rec.19/5 (appendix 3)***	***OSPAR*** ***chemicals of priority action (2007 update)***	***WFD***	***Dir. 76/464*** ***Pertinent daughter directive or amendment of 76/769/EEC***	***Stockholm convention (R=regulated; C=candidate)***
Endrin	X	X		X	Dir. 88/347	R
Isodrin	X	X	X	X	Dir. 88/347	
Carbontetrachloride				X	Dir. 86/280	
Tetrachloroethylene (perchloroethylene)				X	Dir. 90/415	
Trichloroethylene				X	Dir. 90/415	
PCB	X	X	X			R
PCDD/F	X	X	X			R
Chlordane	X	X				R
Mirex	X	X				R
Toxaphene	X	X				R
heptachlor	X	X				R
chlordecone	X	X				C
PFOS			X		2006/122/ ECOF	C
Phenols (as total C)		X				
Xylenes		X	X (musk xylene)			
Dibutylphthalate		X	X			
Chlordimeform		X				
Acrylonitrile		X				
1,2-Dibromoethane		X				
2,4,5-T		X				
Aramite		X				
Kelevan		X				

Table 5 - regulations

Substance Name	Aarhus (CLRTAP)	HELCOM rec.19/5 (appendix 3)	OSPAR chemicals of priority action (2007 update)	WFD	Dir. 76/464 Pertinent daughter directive or amendment of 76/769/EEC	Stockholm convention (R=regulated; C=candidate)
Isobenzane		X				
Morfamquat		X				
Nitrophen		X				
Quintozene		X				
dicofol			X			
tetrabromobisphenol A (TBBP-A)			X			
methoxychlor			X			
2,4,6-tri-tert-butylphenol			X			
4-(dimethylbutylamino)diphenylamin (6PPD)			X			
clotrimazole			X			
diosgenin						
PCT (mixtures)		X				
PBB		X (hexabromobiphenyl)	X			C (hexabromobiphenyl)
Hexabromocyclododecane (HBCDD)			X			C
Organic mercury compounds			X			
Organic lead compounds			X			
Neodecanoic acid			X			
Ethenyl ester			X			

Table 6 - studies, emission inventories, monitoring

Substance Name	Pesticide[1]	EPER	E-PRTR	RARs[2]	EMEP emiss.	COMMPS[3]	Eurochlor[4]	use(s)[5]:	year of ban	notes
Alachlor	O		X			2		P	2006	
Anthracene			X	R		2		I		
Atrazine	O		X			2		P	2004	allowed until 2007 with restrictions
Benzene		X (as BTEX)	X	D		2		I, B		
Brominated diphenylethers		X	X	D		0		I	2003	
C_{10}-$_{13}$-chloroalkanes		X	X	R		0		I	2004	allowed use in conc. <1%
Chlorfenvinphos	O		X			1		P	2002	
Chlorpyrifos	X		X			1		P		
1,2-Dichloroethane	*	X	X			1	M	I		
Dichloromethane		X	X			1	M	I		
Di(2-ethylhexyl)phthalate (DEHP)			X			2		I		
Diuron	X		X			2		P	2007	
Endosulfan	O		X			2		P	2005	
Fluoranthene			X			2		B		
Hexachlorobenzene	*	X	X		X	2	R	P	2001	
Hexachlorobutadiene		X	X			2	M	I		under phase out
Hexachlorocyclohexane	*	X	X		X	2		P		under phase out
Isoproturon	X		X			2		P		
Naphthalene			X	R		2		I		
Nonylphenols			X	R		2		I	2003	
Octylphenols			X			0		I		
Pentachlorobenzene			X			2	R	I		
Pentachlorophenol		X	X			2	M	I	1999	derogations
Polyaromatic hydrocarbons		X	X		X	0		B		
(Benzo(a)pyrene),			X			2				
(Benzo(b)fluoranthene),			X			2				
(Benzo(g,h,i)perylene),			X			2				

Table 6 - studies, emission inventories, monitoring

Substance Name	Pesticide[1]	EPER	E-PRTR	RARs[2]	EMEP emiss.	COMMPS[3]	Eurochlor[4]	use(s)[5]:	year of ban	notes
(Benzo(k)fluoranthene),			X			2				
(Indeno(1,2,3-cd)pyrene)			X			2				
Simazine	O		X			2		P	2005	
Tributyltin compounds		X	X			2		I		antofouling, wood preservative…
Trichlorobenzenes		X	X	R		2	M	I		
Trichloromethane (Chloroform)		X	X			1	M, R	I		
Trifluralin	O		X			2		P		
DDT	*		X		X	2		P	1986	
Aldrin	*		X			2		P	1988	
Dieldrin	*		X			2		P	1988	
Endrin	*		X			2		P	1988	
Isodrin	*		X			2		P	1986	
Carbontetrachloride			X			1	M	I	1986	
Tetrachloroethylene (perchloroethylene)		X	X			1	M	I	1990	
Trichloroethylene		X	X			2	M	I	1990	
PCB		X	X		X			I	2005	previous ban in different EU countries
PCDD/F		X	X		X			B		
Chlordane	*		X					P		
Mirex	*		X					P		
Toxaphene	*		X					P		
heptachlor	*		X					P		
chlordecone	*		X					P		
PFOS								I	2006	derogations until 2008
Phenols (as total C)		X	X							
Toluene		X (as BTEX)	X							
Vinyl chloride			X							
Ethyl benzene		X (as BTEX)	X							
Ethylene oxide			X							

Table 6 - studies, emission inventories, monitoring

Substance Name	Pesticide[1]	EPER	E-PRTR	RARs[2]	EMEP emiss.	COMMPS[3]	Eurochlor[4]	use(s)[5]:	year of ban	notes
Triphenyltin and compounds			X							
Xylenes		X (as BTEX)	X							
Hydrogen cyanide (HCN)		X	X							
Cyanides (as total CN)		X	X							
Tetrachloromethane (TCM)			X							
1,1,1-trichloroethane		X	X							
1,1,2,2-tetrachloroethane			X							
Aramite	(never notified)									
Kelevan	(never notified)									
Isobenzane										
Morfamquat	*									
Nitrophen										
Quintozene	*									
dicofol	*									
methoxychlor	O									

[1] *(X=annex 1 dir. 91/414; O=out of annex 1 dir. 91/414; *=banned)*
[2] *(R) or draft RARs(D)*
[3] *data (0=no data, 1=water only; 2= water + sediments)*
[4] *report [R] or marine risk assessment [M]*
[5] *P=pesticide; I=industrial chemical; B=by-product; =human pharmaceutical; VP=veterinary pharmaceutical*

7. The assessment of priority chemicals: example with three pilot substances

7.1 Introduction

The assessment of chemicals of interest is typically performed using fate and transport models, which use chemical emission figures and convert them into predicted environmental concentrations (PECs) and flows. Unfortunately, most of the times emissions are neither known nor easy to estimate, not even at the level of orders of magnitude.

Emissions, environmental concentrations and environmental processes producing the removal of chemicals from a given medium (air, water, soil, sediments…) are mutually connected.

Most of the times, when assessing the spatial distribution of chemicals, it is not possible to make a direct prediction of environmental concentrations, because emissions are not known. An essential step is to take into consideration monitoring data, in what is sometimes referred to as "joint interpretation of model results and data". A systematic way to do so is to perform both "direct" and "inverse"modelling, i.e. to start iteratively once from emission estimates to predict concentrations, and once from observed concentrations to back-calculate emissions (Figure 9). In this report, we discuss these concepts and the limitations currently hampering an extensive and reliable assessment of chemicals at the European scale, having this concept in mind.

The results presented here are a condensation of more extended papers, quoted throughout the document, to which the reader is referred for further details, scientific discussion, and additional references.

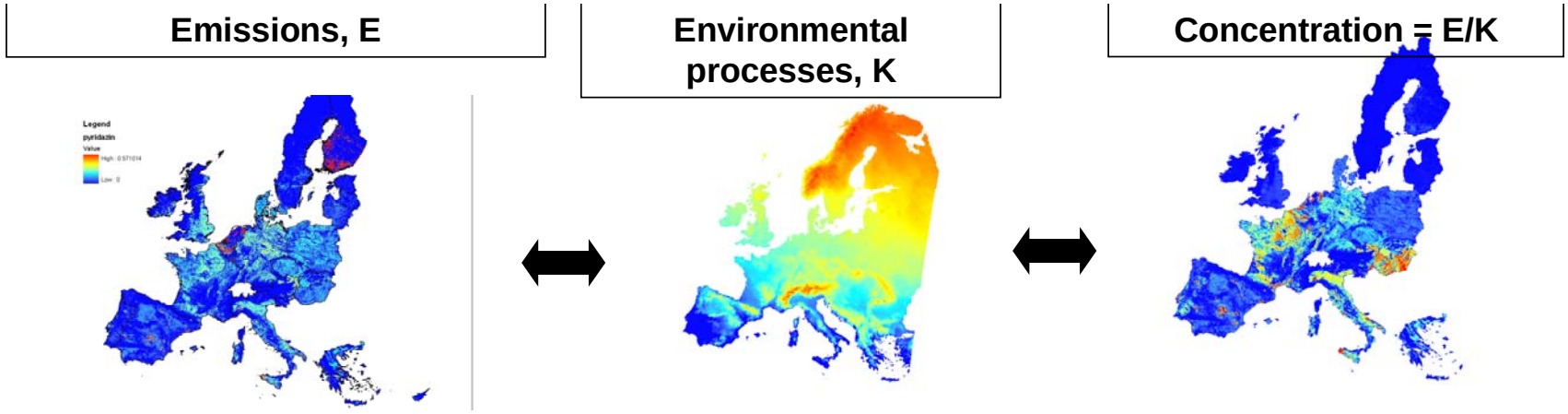
7.2 Scope

In the present report we describe the data available and methods applicable to characterize the spatial distribution of three example chemicals of concern for coastal waters in Europe, with reference to the baseline year (representative of present conditions). The baseline year is 2007 for PFOS, 2003 for Trifluralin and 2005 for Lindane. This is due to a number of limitations on available data, which suggest considering those years as a reference in order to better develop retrospective and prospective scenarios.

7.3 Emissions and loads for the baseline scenario: Trifluralin

No data on the use and emissions to the environment of individual pesticides exist at European level, and Trifluralin is no exception. The only possibility to map pesticide emissions in Europe relies presently on data available on the use of classes of chemical substances, with reference to the years 1992-2003 (EUROSTAT, 2007). Based on these data and the Corine Land Cover 2000 map (http://terrestrial.eionet.europa.eu/CLC2000), Pistocchi et al., 2009, propose a method to estimate emissions of individual substances, by simply assuming that the whole class of chemicals in use is composed, each time, by

one single substance. This method is clearly simplistic and grounds on the argument that, if a chemical class is used, then it is likely that a single substance from that class is used at a specific location, as the other represent substitutes. This approach leads to a systematic overestimation of the use of any chemical; the more chemicals the class of substances includes, the larger will be the overestimation. E.g., for dinitroaniline herbicides (8 chemicals including trifluralin) EUROSTAT (2007) reports the use of 6182 tonnes for 2003. Figure 10 provides a scheme of the procedure for the estimation of emissions.



Where do chemicals go? **(direct modelling)**

From known emissions, estimate concentrations

-> is there a problem with substances in use?
-> analyze scenarios of different emissions (what…if…?)
-> identification of possible problem areas
-> identification of monitoring needs

Where do chemicals come from? **(inverse modelling)**

From known concentrations, estimate emissions

-> what are the conditions determining environmental concentrations of concern?
-> identify sources of contamination
-> support in targeting emissions (restriction, ban…)

Figure 9 – direct and inverse modeling

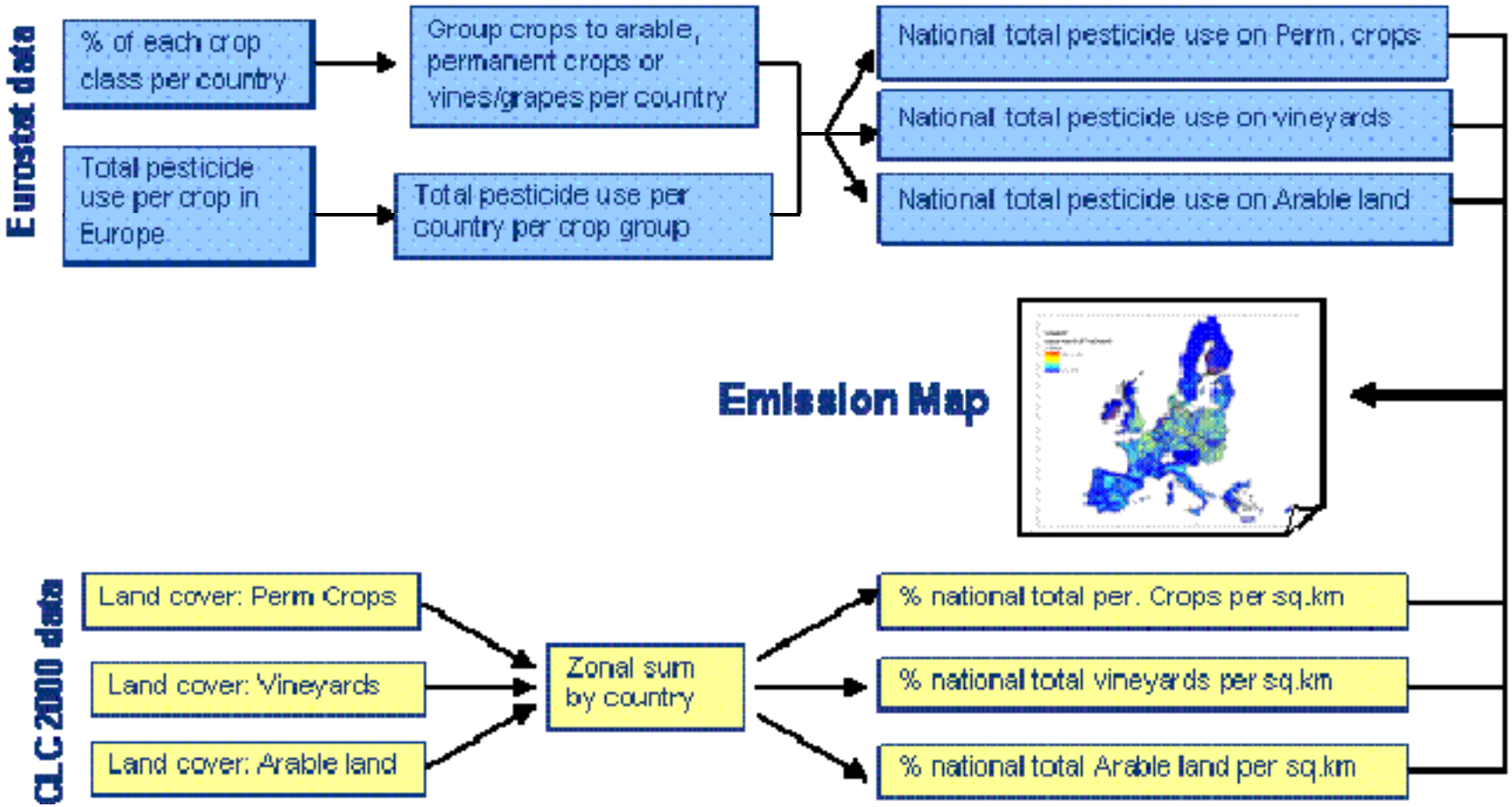


Figure 10 – flow chart for the calculation of the emission map (Pistocchi et al., 2009)

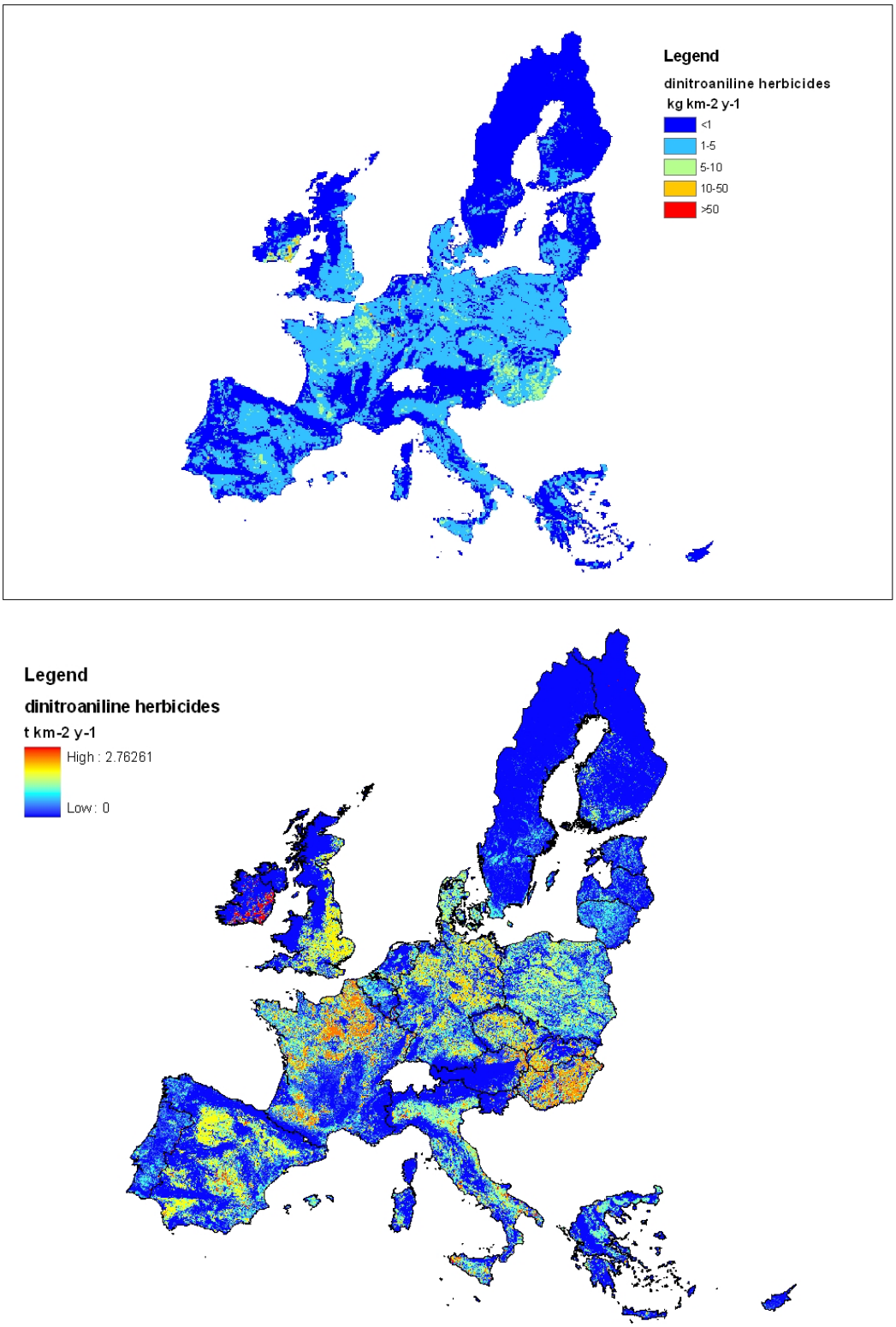


Figure 11 – use of dinitroaniline herbicides: above, classified legend; below, continuous (stretched) legend

Based on the emission estimate of Figure 11, it is possible to compute concentrations of trifluralin in different media according to Pistocchi and Bidoglio, 2009, particularly, mass in soil (Figure 12) and runoff load to surface water (Figure 13) are of interest.

In addition to runoff load, direct losses should be accounted for. These include wind drift, dripping from distribution equipment and all losses unaccounted for by a soil water and chemical balance model; they usually account for about 1% of use (emissions) and represent, in the case of trifluralin, a larger portion of loads than runoff. Under the assumption that direct losses are 1% of use,

Figure 14 shows the spatial distribution of loads to European coastal waters.
This method of estimation has proven to be correct in orders of magnitude, but to suffer from the lack of knowledge of emissions which hampers any possibility to predict reliably the spatial distribution of concentrations.

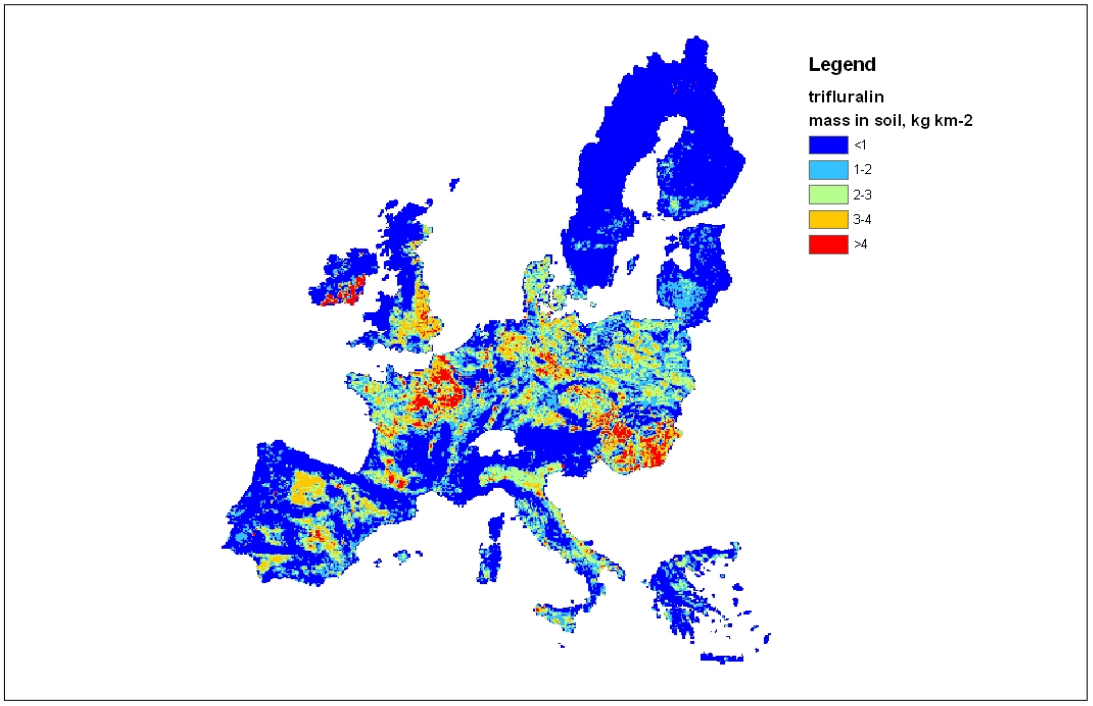


Figure 12 – mass of Trifluralin in soil, 2003

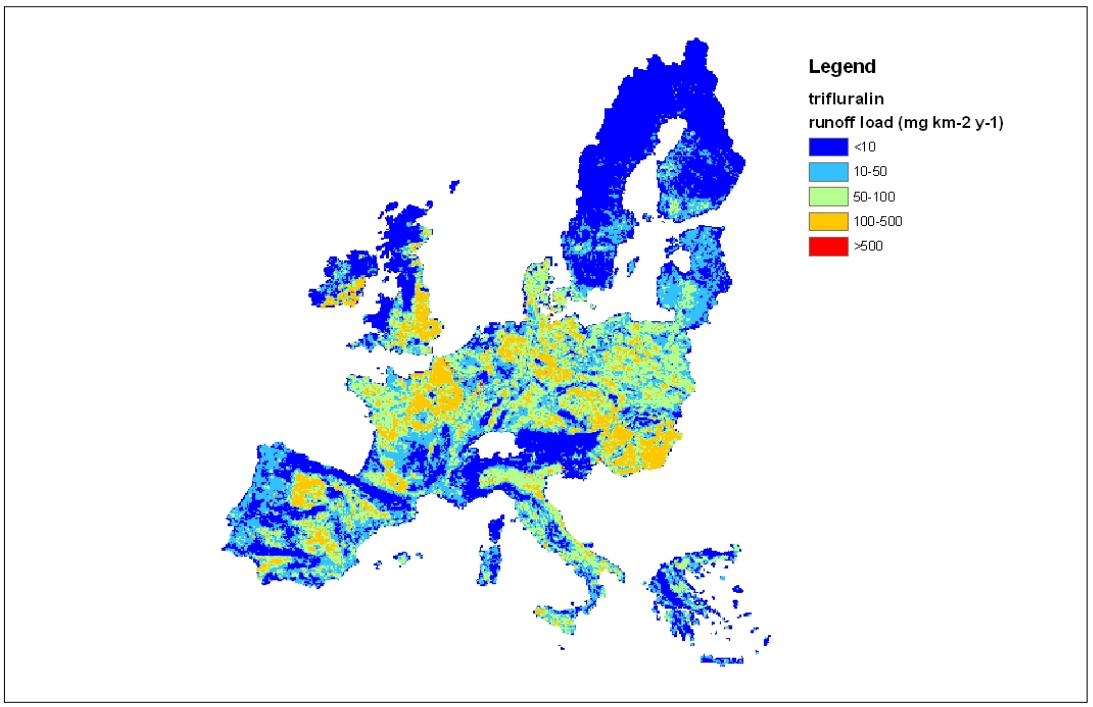


Figure 13 – loads of trifluralin through runoff, 2003

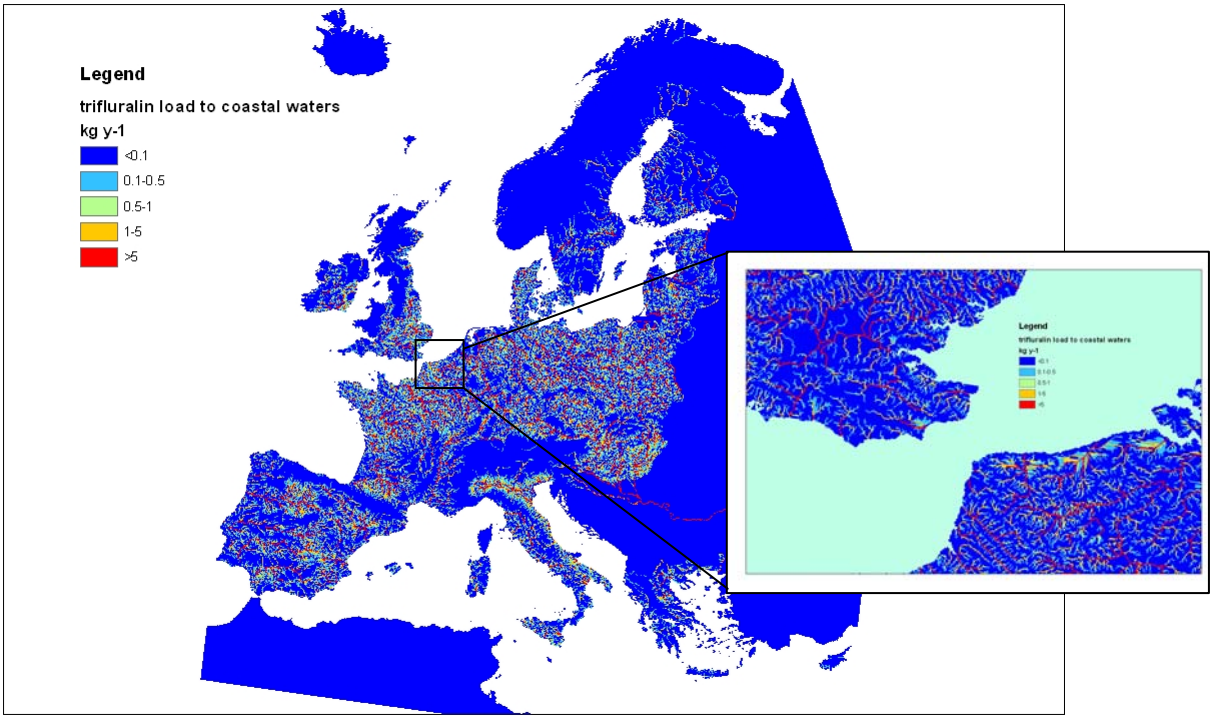


Figure 14- loads of trifluralin assuming direct losses equal to 1% of use.

7.4 Emissions and loads for the baseline scenario: PFOS

Only limited information is available on sources, volumes, and emissions of PFOS, although more is known about perfluorocarboxylic acids (PFCAs) (Paul et al., 2009). Direct industrial emissions are supposed to have ceased because of the phase-out of the substance in Europe in December 2007 (in most applications). However, this molecule is very persistent and continues to be released from mostly "indirect" wide-dispersive uses (i.e., breakdown in the environment from PFOS-derivatives). The persistence of the substance and its use pattern, which is relatively constant throughout the year, enable estimating loads to coastal waters by flow-accumulation of unit emissions based on population density, as shown in Pistocchi and Loos, 2009. There is a clear correlation between population in a catchment and mass discharge of PFOS (Figure 15), as highlighted by an Europe-wide sampling campaign (Loos et al., 2009).

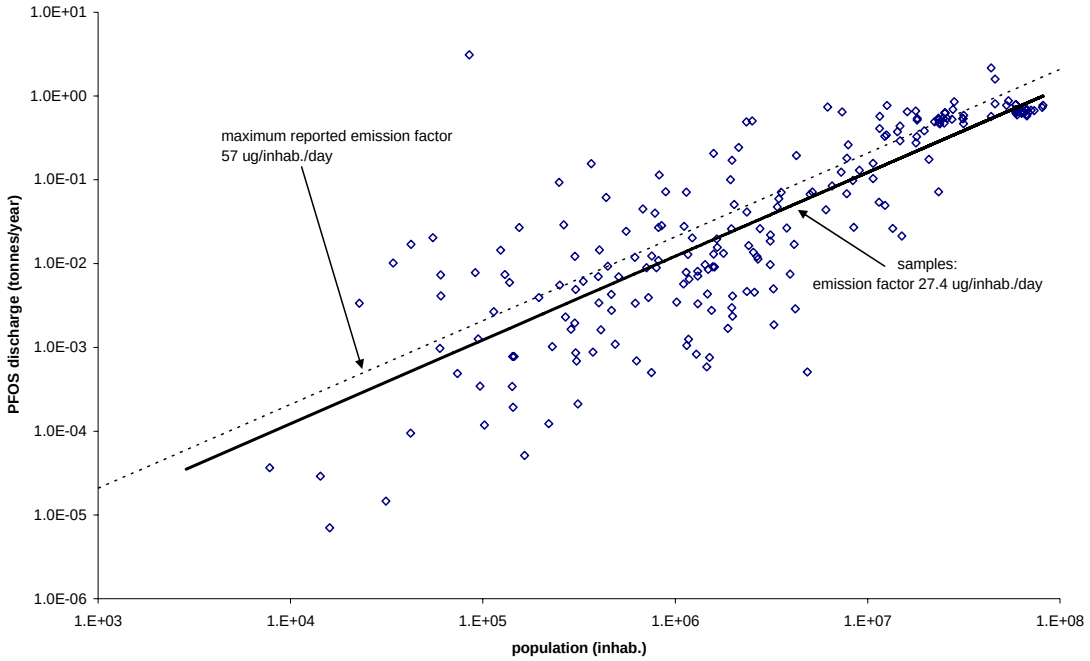


Figure 15 - linear scatter plots of observed PFOS discharges in European rivers with population in the catchment upstream (from Pistocchi and Loos, 2009).

By using the emission factor highlighted in Figure 15 (27.4 µg/inhabitant/day), it is possible to compute the emission map as shown in
Figure 16. The map reflects the situation at the date of sampling (during year 2007). Overall, by using a log-linear model, PFOS discharges along the whole European river network to coastal areas in Europe have been estimated for the year 2007 to be in the order of 20 tons (Pistocchi and Loos, 2009). The reader is referred to the latter publication for further details also concerning the evaluation of the inverse modelling approach.

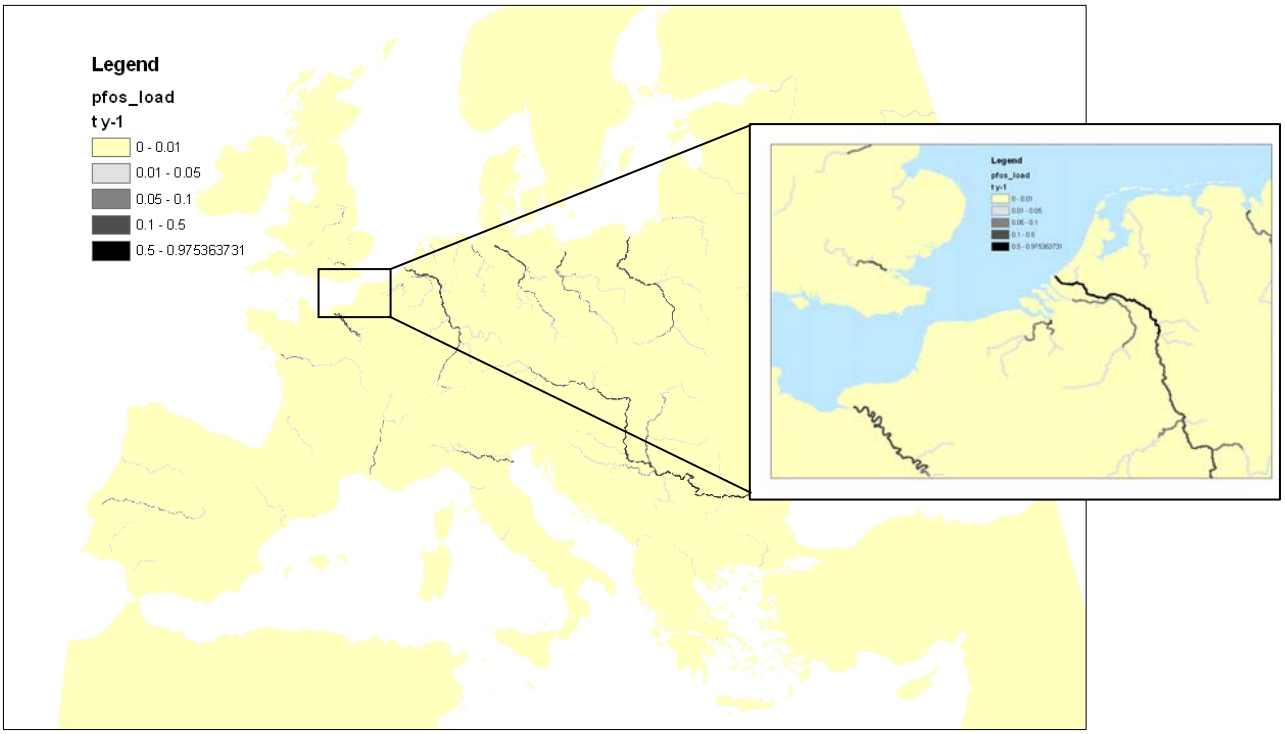


Figure 16 – loads of PFOS to European coastal waters (samples taken in 2007). From Pistocchi and Loos, 2009, modified.

7.5 Emissions and loads for the baseline scenario: Lindane

Lindane (or gamma-hexachlorocyclohexane,γ-HCH) is a chemical of interest for many years, both as a subject of scientific investigation and as a regulated substance, which is currently banned for agricultural usage in Europe, and listed as a priority substance under the water framework directive.
Lindane emissions are estimated by EMEP (www.emep.int) in the framework of the reporting and analysis of chemical data under the protocol on long range transport of chemicals of the Montreal convention. In that context, focus is primarily on emissions to the atmosphere, while emissions to soil and waters have historically accounted for significant percentages of the total environmental emissions.
Lindane is relatively well monitored, and provides an interesting case study for the evaluation of our capability to actually predict the fate of chemical substances in Europe. In this report, results are presented which are discussed more in detail in Vizcaino and Pistocchi, 2009a, to which the reader is referred for further information.
Atmospheric emission estimates for lindane in Europe are available from EMEP. From these estimates, total emissions can be calculated assuming emissions to air are 17.5% of the total (see the discussion in Vizcaino and Pistocchi, 2009b). Using the MAPPE modelling approach (Pistocchi, 2005, 2008) emissions are used to compute maps of air, soil and water concentration of Lindane in Europe. The atmospheric component, which is less relevant for the purposes of this study, is presented and discussed in Vizcaino and Pistocchi, 2009b.
Concerning soil concentrations in 1995 (Figure 17), the emission estimates from EMEP point at high values in France and the UK deriving from high emissions. The higher values of predicted soil concentration are in line with the limited observations available at one polluted site in Germany for 1995. Lindane is relatively soluble, and concentrations in water follow the same pattern as in soil (Figure 18). For the water compartment, predicted concentrations match observations to a satisfactory extent in 1995 (Figure 18).

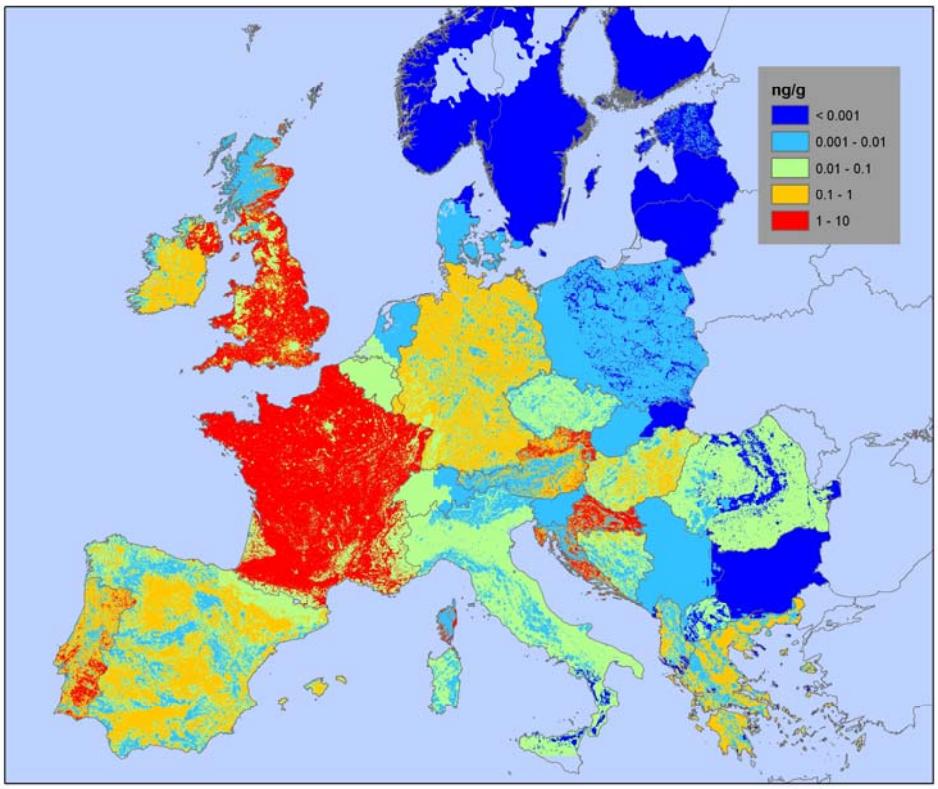
Table 7. Atmospheric total emissions per country for 1995 and 2005 (left) and total emissions per country to all media (right) used for the computations, derived from information used for the computations of the MSCE-POP model (http://www.msceast.org/). From Vizcaino and Pistocchi, 2009b

γ-HCH emissions, tonnes	1995 atm	2005 atm	1995 tot	2005 tot
Albania	0.463	0.123	2.645	0.703
Armenia	0.030	0	0.171	0.000
Austria	8.1	0	46.286	0.000
Azerbaijan	0.113	0	0.6464	0.000
Belarus	0.003	0	0.017	0.000
Belgium	0.165	0.168	0.9437	0.960
Bosnia&Herzegovina	0.515	0.115	2.943	0.657
Bulgaria	0	0	0	0.000
Croatia	12	3.2	68.571	18.286
Cyprus	0	0	0	0.000
Czech Republic	0.319	0	1.822	0.000
Denmark	0	0	0	0.000
Estonia	0.005	0	0.029	0.000
Finland	0	0	0	0.000

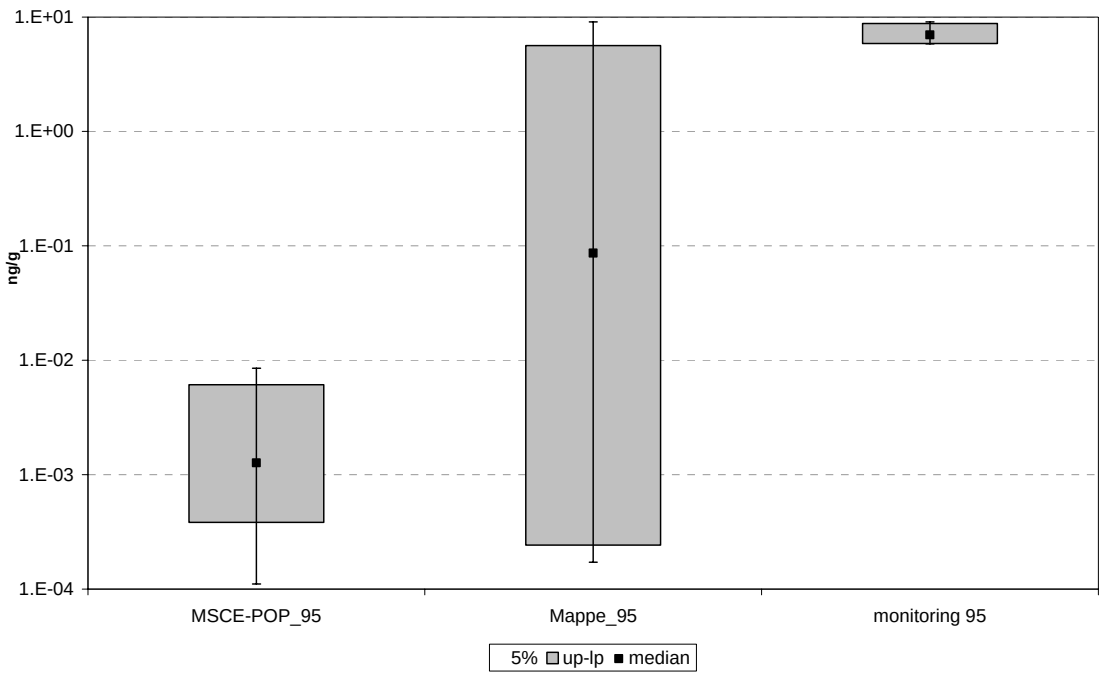
France	560	40	3200	228.571
Georgia	0.095	0	0.543	0.000
Germany	13	0	74.286	0.000
Greece	5.9	2.4	33.714	13.714
Hungary	1.7	0	9.714	0.000
Iceland	0	0	0	0.000
Ireland	2.2	0	12.571	0.000
Italy	2.2	2.2	12.571	12.571
Kazakhstan	0.446	0	2.549	0.000
Latvia	0.002	0	0.011	0.000
Lithuania	0.003	0	0.017	0.000
Luxembourg	0.151	0	0.869	0.000
Netherlands	0	0	0	0.000
Norway	0	0	0	0.000
Poland	0.283	0	1.617	0.000
Portugal	11	7.7	62.857	44.000
Moldova	0	0	0	0.000
Romania	2.3	1.1	13.143	6.286
Russia	132	0	754.286	0.000
Serbia&Montenegro	1.5	0.51	8.571	2.914
Slovakia	0	0	0	0.000
Slovenia	0	0	0	0.000
Spain	9.5	10	54.857	57.143
Sweden	0	0	0	0.000
Switzerland	0	0	0	0.000
The FYR of Macedonia	0.063	0.087	0.36	0.497
Turkey	12	12	68.571	68.571
Ukraine	9.1	0	52	0.000
United Kingdom	59	13	280	74.286
Europe	**845**	**93**	**4765.714**	**531.429**

For the year 2005, if one neglects direct emissions to soil and water and considers only emissions to the atmosphere as reported by EMEP (Table 7), soil concentrations appear to be much more evenly distributed as they arise from atmospheric deposition only (Figure 20). This yields to a trend in underestimation of concentrations with respect to the EMEPMSCE-POP model. Concentrations in water predicted under the assumption of emissions to the atmosphere only (Figure 21 A) appear to be too low with respect to monitored data (Figure 21 B).

In order to better understand the source of the underestimation, actual emissions of lindane to water were computed for each of the monitored catchments by multiplying observed lindane concentrations by the water discharge considered by the model. This yielded to a map of "observed" lindane loads, in a similar way to what done for PFOS (Pistocchi and Loos, 2009), as shown in Figure 22. By assuming that lindane is conservative in water (which is acceptable given its persistence and the generally short residence time of European surface waters), these loads provide a range of variation of estimated emissions to water, which compare favourably with the emissions to water estimated from emissions to the atmosphere in 2005, by applying a proportion of 2.5 : 17.5 between the two as further discussed in Vizcaino and Pistocchi, 2009b (Figure 23). This indicates that direct emissions to water, or emissions to soils eventually leaching to the stream network, are still very likely to occur in 2005 despite the ban or restriction of lindane. Indeed, if one considers emissions for 2005 to air, water and soil to be in the same proportion 17.5 : 2.5: 80 as in 1995, the predicted concentrations appear to be in the correct ranges, although the indirect estimation based on EMEP estimates of air emissions yields some discrepancies (Figure 24). Further discussion is found in Vizcaino and Pistocchi, 2009b.



A



B

Figure 17 - (A) Estimated concentrations of γ-HCH in soils for the year 1995, in (ng/g); (B) comparison of ranges of concentrations against the EMEP MSCE-POP model and monitoring data, from Vizcaino and Pistocchi, 2009b. Details on the monitored concentrations in 1995, that represent polluted sites, are provided in Vizcaino and Pistocchi, 2009b.

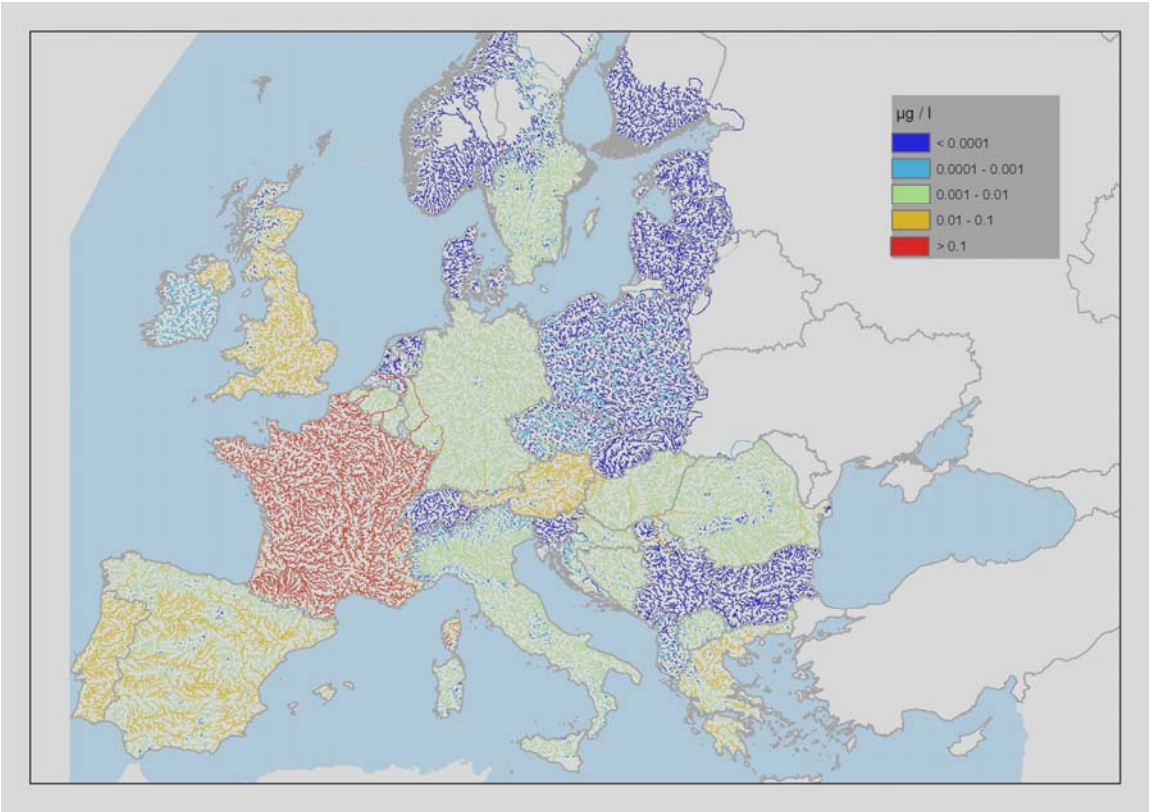


Figure 18- Estimated concentrations of γ-HCH in continental surface waters for the year 1995 in (µg/l). From Vizcaino and Pistocchi, 2009b.

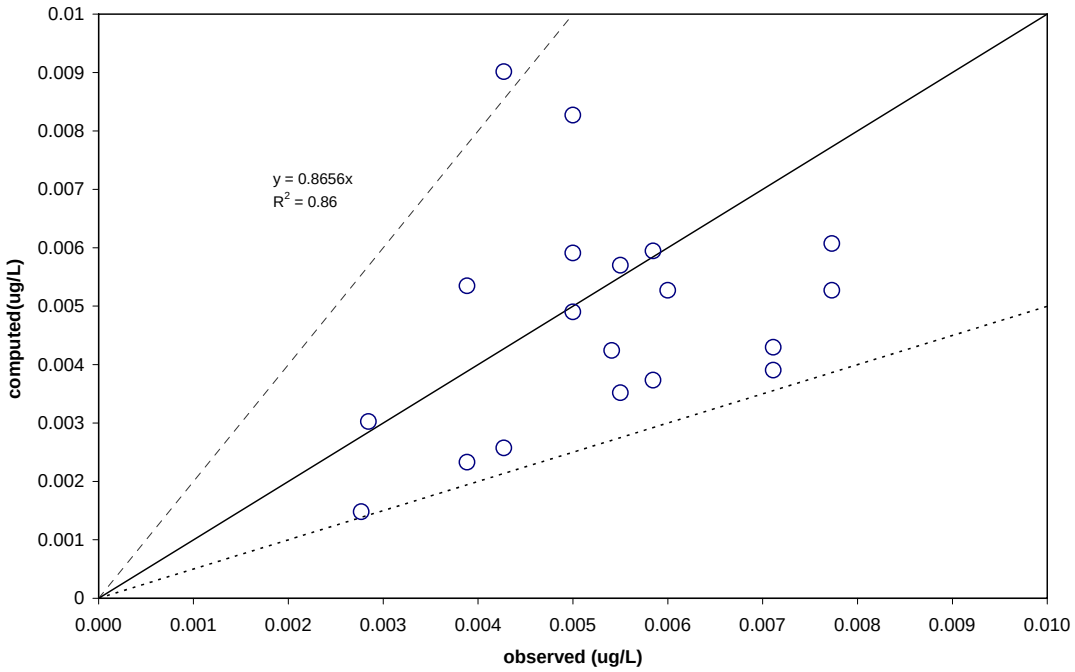
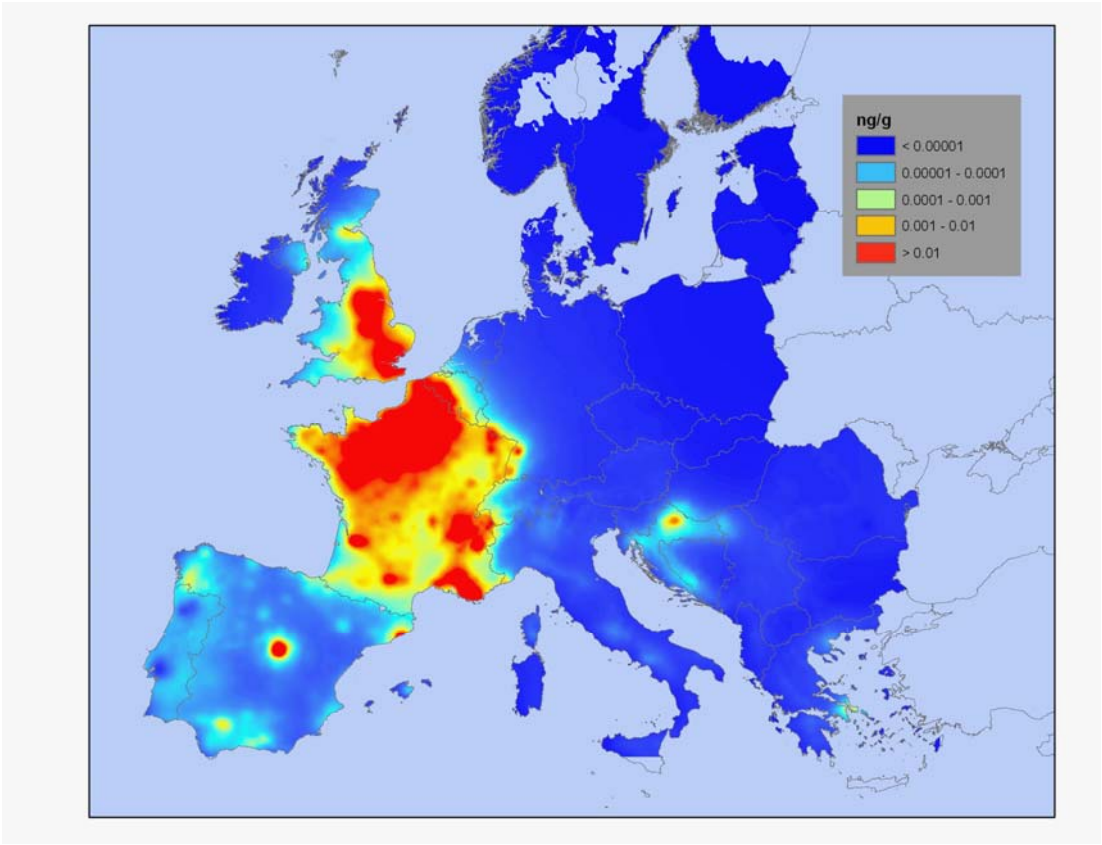
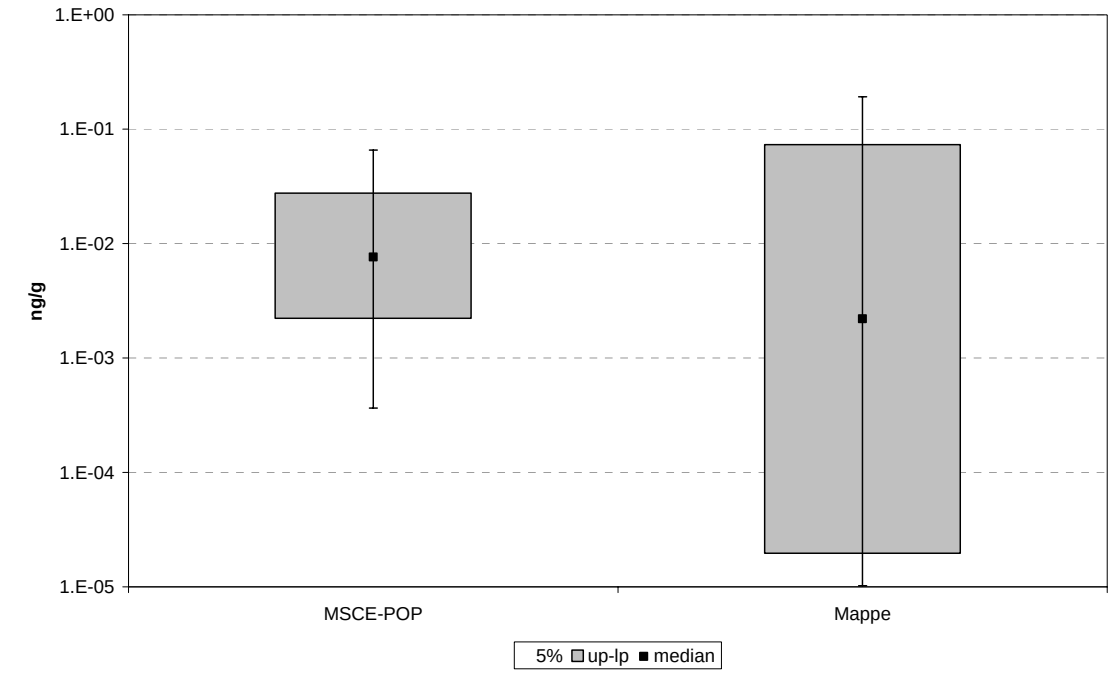


Figure 19- Comparison of concentration in water of γ-HCH in 1995 in µg/l predicted by MAPPE and observed in monitoring stations along the Elbe river in Germany (1:1 line and a factor 2 discrepancy lines are displayed). From Vizcaino and Pistocchi, 2009b.

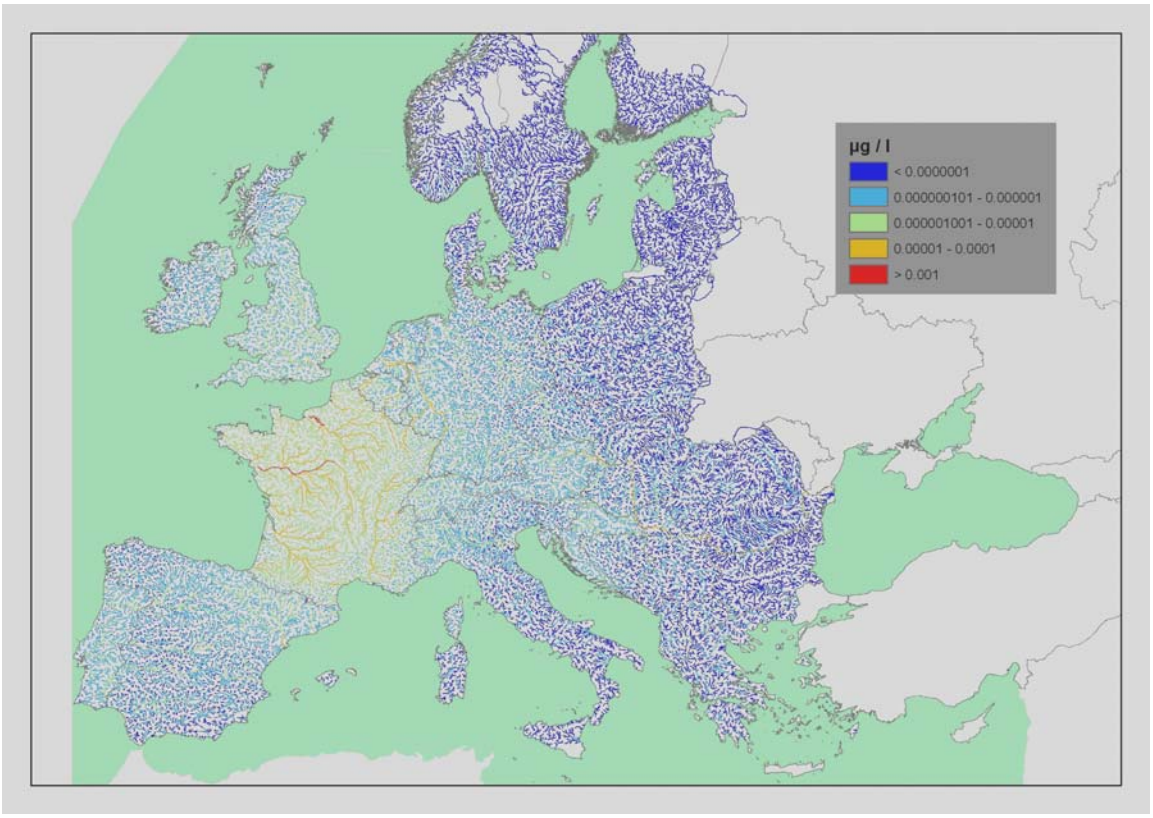


A



B

Figure 20 - (A) Estimated concentrations of γ-HCH in soils for the year 2005, in (ng/g); (B) comparison of ranges of concentrations against the EMEP MSCE-POP model. From Vizcaino and Pistocchi, 2009b.



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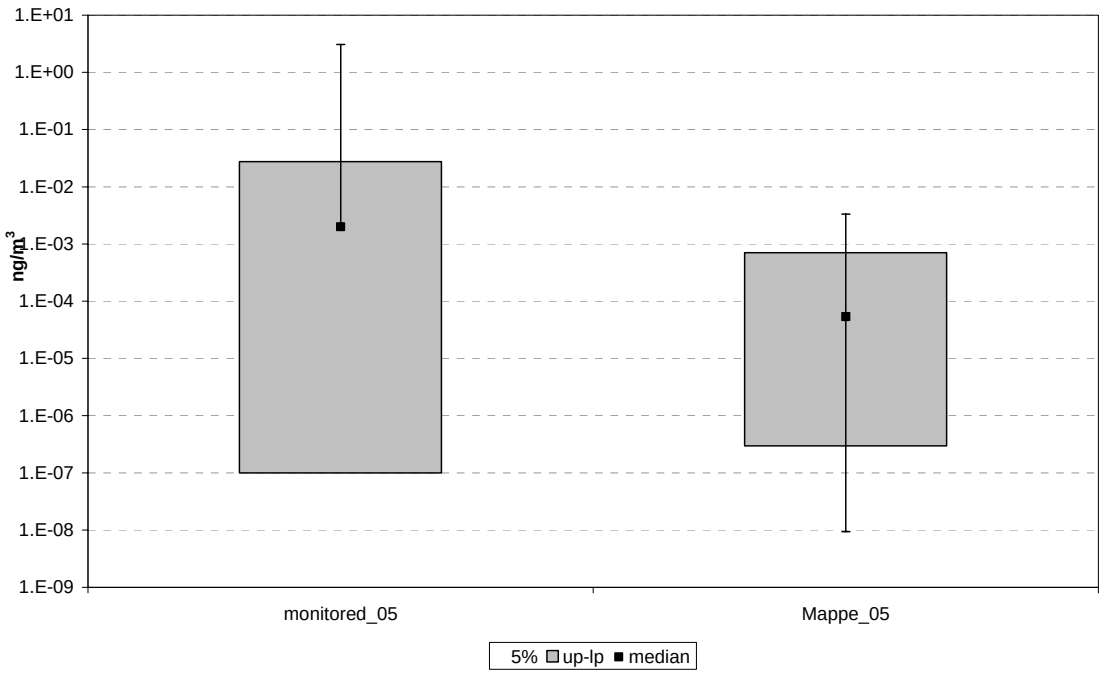

B

Figure 21 - (A) Estimated concentrations of γ-HCH in continental surface waters for the year 2005 in (µg/l); (B) comparison of ranges of concentrations. From Vizcaino and Pistocchi, 2009b.

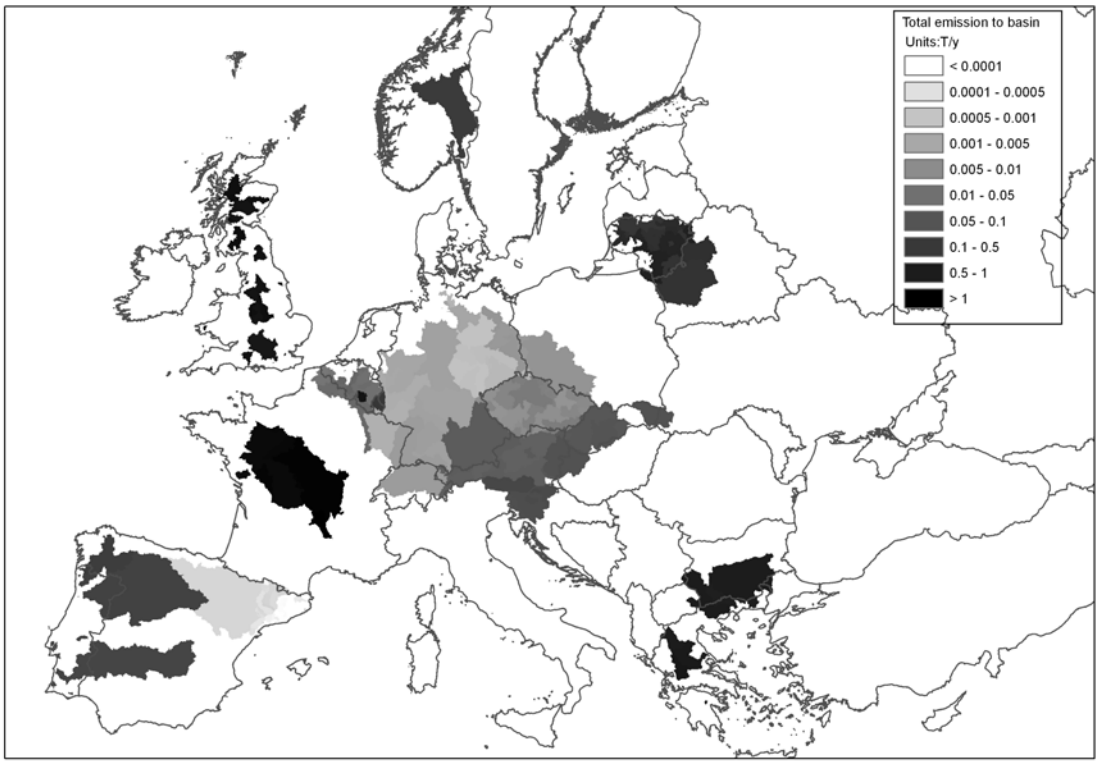

Figure 22 - Estimated emissions of γ-HCH to basins for 2005. From Vizcaino and Pistocchi, 2009b.

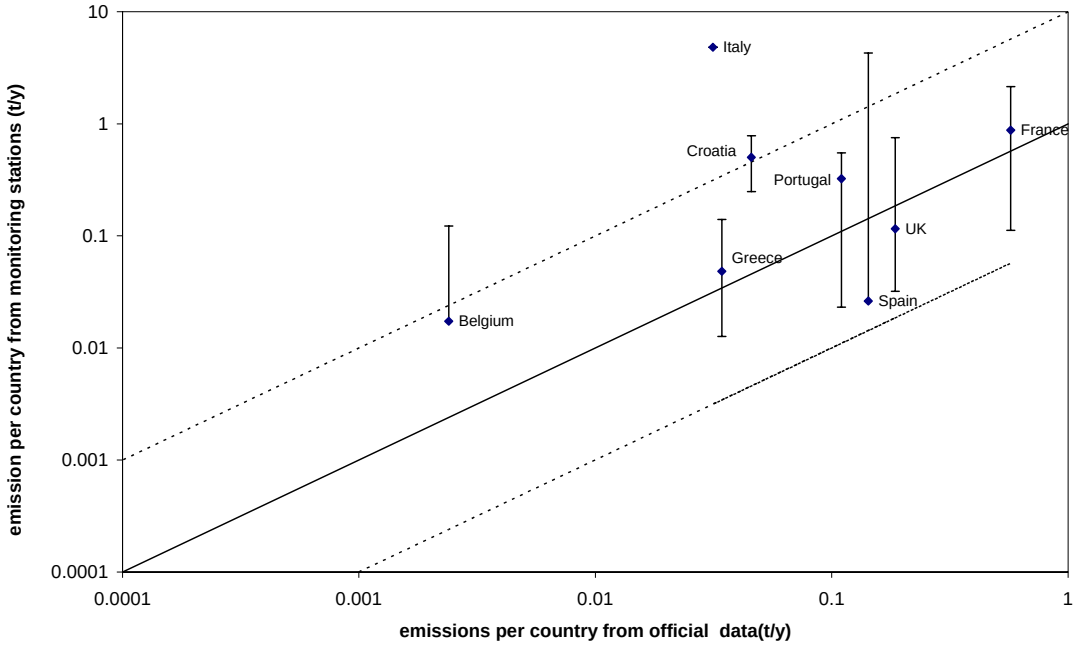

Figure 23 - Comparison of total emissions of γ-HCH to water per country estimated from data of concentration in monitoring stations and total emission to water per country, estimated from data of total emissions in 2005 (Table 7). 1:1 and a factor 10 lines are displayed. From Vizcaino and Pistocchi, 2009b.

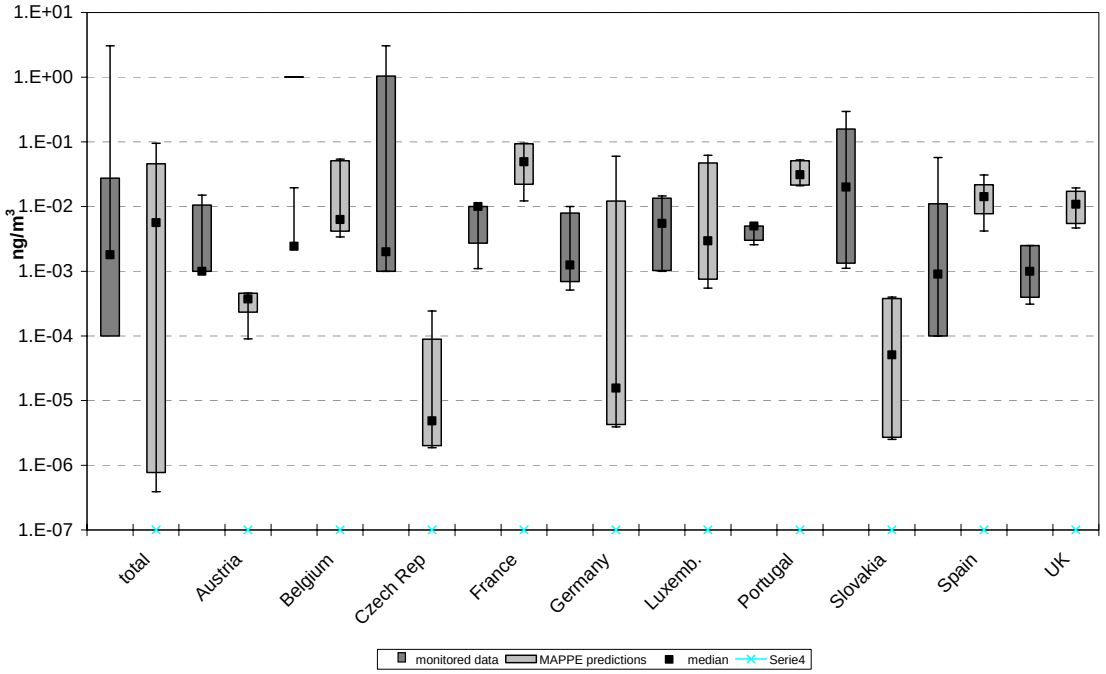

Figure 24 - Comparison of values of concentration in water predicted with the MAPPE model, according to the emission estimated in the same proportion (to soil, water and air) as in 1995, and values of concentration measured in the monitoring stations. From Vizcaino and Pistocchi, 2009b.

7.6 Conclusions and perspectives

The research presented here yields an understanding of our current capabilities to predict the concentrations and loads of chemical contaminants in Europe. A general observation that needs to be done concerns the current knowledge of emissions. These are affected by huge uncertainties, sometimes even in terms of orders of magnitude, and usually also in terms of their spatial distribution.

Pesticides in general, and trifluralin in particular, are roughly known in terms of the total amount used in Europe, and predictions of their environmental concentrations generally prove to be correct within one order of magnitude based on the available information on their physico-chemical properties. In order to predict their spatial and temporal distribution, however, massive efforts are still required in order to achieve a reliable spatial distribution of emissions, from which, consequently, it is expected that environmental concentrations and loads may be predicted reliably.

Substances subject to widespread use, such as PFOS, are best predicted by inverse modelling based on measured concentrations. An a-priori estimation of emissions is presently not feasible due to lacking information. Similar issues arise for chemicals such as pharmaceuticals and biocides, household pesticides, and practically all emerging pollutants unless deriving from specific industrial processes.

In the case of "historical" contaminants such as Lindane, although in theory there is a good basis for theoretical emission estimation and consequent environmental fate simulation, in practice there are still broad areas where knowledge is lacking. Among them, particularly, emissions represent the critical piece of information.

On the other hand, when emissions are provided with sufficient realism, predictions of the spatial distribution of chemicals are sufficiently accurate, at least for general policy support: this means that, for many substances, our conceptual understanding and parametrization of environmental drivers of chemical fate is sufficient at least for screening and general reasoning. Therefore, it can be recommended that in the future, pending better estimates of chemical emissions, the spatial distributions of environmental parameters be used to derive frequency distributions of environmental removal rates, through which to support the reasoning on trends of chemical concentrations and fluxes in lumped, and not in spatially explicit terms.

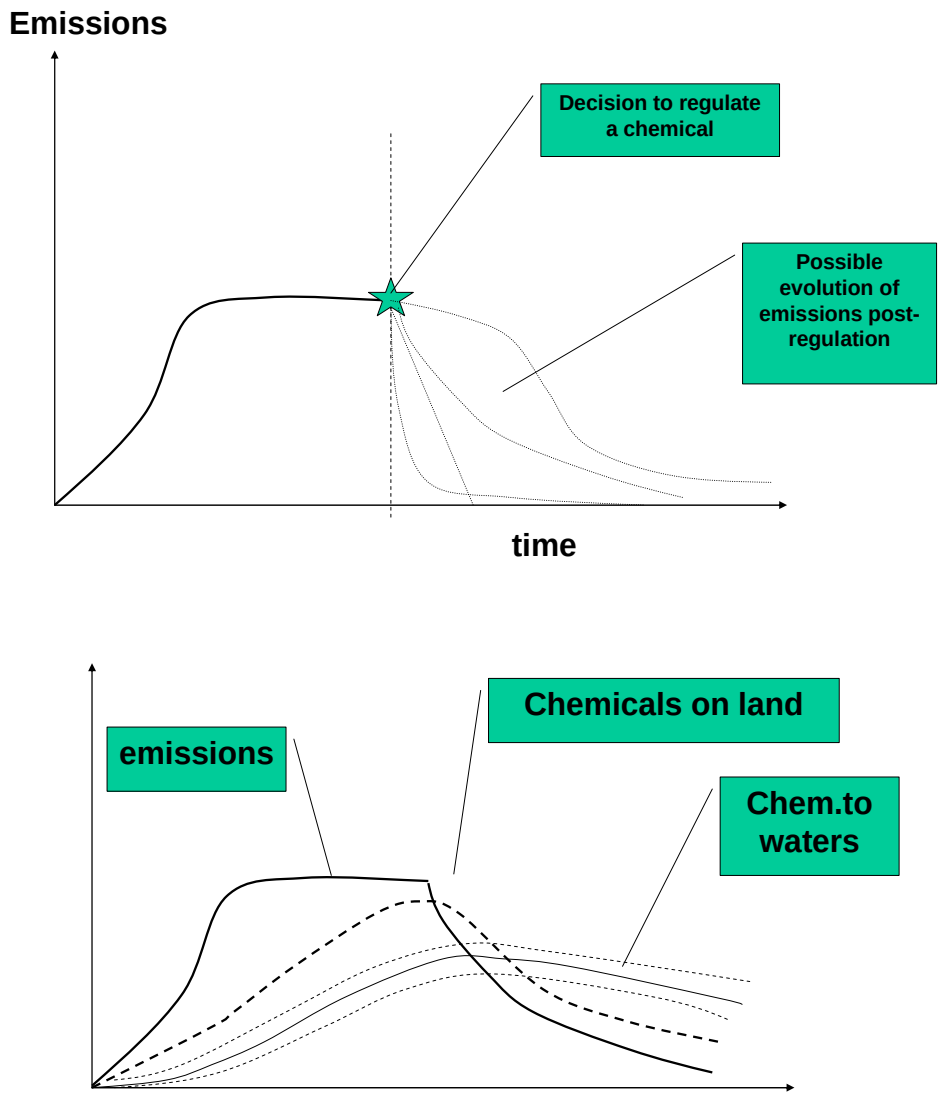

Figure 25 – conceptual scheme of the reasoning for the evaluation of scenarios

Conceptually, one should clarify the type of emission trend in time and the likely order of magnitude of emissions. The variability of environmental parameters, hence intra-media and inter-media transfer rate, provide the range of variability of the "environmental breakthrough curves" of a chemical, following a given emission scenario (as shown schematically in Figure 25). The assessment of scenarios will then necessarily start from the assessment of a lumped emission history, neglecting, given the present state of knowledge, the apportionment of emissions to sources in space.

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Abstract

In this report we present a survey of existing information for the assessment of loads of hazardous substances to the European coastal waters. Based on the information available, we select three example substances (PFOS, trifluralin and lindane) for which we perform an assessment of the baseline conditions and (limited) retrospective analysis using direct and inverse modeling. We also suggest criteria and methods to assess future scenarios of chemical loads in response to legislative provisions and accounting for the physico-chemical properties of the substances, based on the use of lumped models but accounting for the spatial variability of environmental processes and emissions.

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