

DEVELOPMENT OF AN INTEGRATED DATABASE FOR THE MANAGEMENT OF ACCIDENTAL SPILLS (DIMAS)

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Introduction

The North Sea is one of the most productive ecosystems in the marine environment, but significant input of toxicants from very diverse sources occurs which may harm this ecosystem. Up till now, little attention has been paid to sea-based sources of pollution (e.g. accidental spills or leakage from platforms). Although most of the public interest has gone to oil spills and the quantity of chemicals transported is substantially less than oil, the potential harm for the marine environment from a given amount of chemicals spilled can be several orders of magnitude greater. Many of the chemicals transported by sea are highly toxic and/or persistent, can bioaccumulate or cause long-term effects. In case of an accident at sea, it is important that accurate information on environmental partitioning, bioavailability, (eco)toxicity is immediately available. A number of databases on physical and chemical properties of chemicals have already been developed, but little attention has been paid to specific issues such as the impact on marine life, environmental fate and bioaccumulation in marine food chains. Most often the interpretation is left to the expert user of the database. Should an accident occur in which substances are discharged into the sea, threatening to be washed up on the beach or even spilled by transportation over land, a prompt reaction to the calamity is essential in order to minimize the potential damage. The choice of effective measures to abate the pollution will depend to a large extent on the direct availability of reliable and up-to-date information on the fate, hazards and risk management procedures to be taken for the spilled product. In this regard it is imperative that all relevant information is made available in a proper format that is easily accessible and interpretable for all stakeholders concerned including the non-expert.

Database development

A tool in which environmental data of specific marine pollutants is made available to a broad range of possible end-users has been developed in the DIMAS project. Since the tool should facilitate and support the decision making in case of an accidental spill, involvement of different stakeholders belonging to different organizational levels was a prerequisite so that specific concerns over the complete chain of command could be taken into account. This was reflected in the composition of the proposed users committee that consisted of representatives of federal and municipal administrations, scientists, port authorities, clean-up and care professionals etc. As such it could be ensured that the developed database is tailored to the needs of the different end-users.

The project itself consisted of 4 consecutive phases:

- Identification and selection of the most important contaminants at the Belgian coast, the Belgian Continental Shelf and the Scheldt Estuary.
- Collection of physico-chemical and ecotoxicological information regarding the selected contaminants.
- Evaluation and interpretation of the gathered data.
- Development of an integrated database with a graphical user interface and modelling of the ecotoxicological data.

Phase 1: Identification and selection of the most important contaminants at the Belgian coast, the Belgian Continental Shelf and the Western Scheldt

The value of an environmental risk assessment depends to a large extent on the availability of reliable and up-to-date information. Since it would have been an enormous task to collect data for all hazardous substances that could be of possible concern to the marine environment, it was deemed necessary to restrict the current project to those substances relevant for the Belgian coast, Belgian Continental Shelf and the Scheldt Estuary that would be of highest concern for immediate action. Thus, in the first phase, the priority contaminants were listed to be included in the database. Selection was performed based on criteria such as bioaccumulation potential, toxicity, persistence, frequency of involvement in accidental spills, frequency of transport over sea and volumes transported. Furthermore, the intrinsic presence of contaminants in ships and the occurrence of contaminants in dumpsites were taken into account. This list was compared with other existing priority lists (OSPAR priority lists, ENECE POP list, EU Water Framework directive etc.) and validated against transport data from harbours. An overview of lists and databases used for selecting substances is given in Fig. 1.

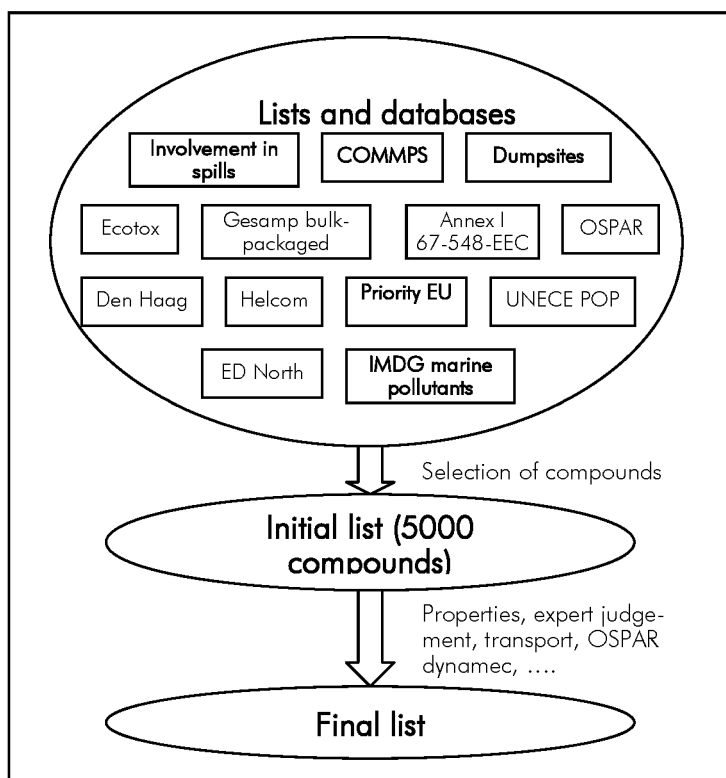


Fig. 1. Selection of substances.

Phase 2: Collection of physico-chemical and ecotoxicological information regarding the selected contaminants

In the second phase an extensive literature search was performed to gather all information necessary for the database. For each of the compounds, data were collected on physico-chemical properties, ecotoxicology, human effects and GESAMP hazard profiles. Most data on acute, subacute and chronic effects at different trophic levels (fish, algae, plants, invertebrates, micro-organisms) were gathered from international scientific literature. Next to peer reviewed literature, existing databases, national and international reports, research programmes etc. were searched.

- Physico-chemical properties were collected from ECB-ESIS (European Chemicals Bureau – official European chemical Substances Information System, containing IUCLID Chemical Data Sheets and Risk Assessment Reports), NSDB (Nordic Substance Database) and peer reviewed literature.
- Ecotoxicological data were mainly gathered from ECB-ESIS, the US-EPA ECOTOX database (US EPA, former AQUIRE database), the ED-North database (database on Endocrine Disruptors in the North Sea), the UGent ECOTOX database (with properties and risk and safety phrases of chemicals transported over the North Sea and ecotoxicological profiles on these chemicals) and peer reviewed literature. Water as well as sediment data were assembled on ecotoxicology. Since marine data were scarce for most compounds, freshwater data were also gathered to allow read across.
- Human toxicological data were mainly gathered from the UGent ECOTOX database and ECB-ESIS.

Phase 3: Evaluation and interpretation of the gathered data

In the third phase quality and relevance of the gathered data were assessed. This was of utmost importance for the data compiled on the effects on marine biota. Therefore, a detailed quality screening of marine data and a rough quality screening of the (less relevant) freshwater data were carried out. The marine data were classified based on the availability of the following information: performance of the tests according to internationally accepted procedures, information on the 'control', information on the test concentration range, availability of information on test characteristics, statistical analysis of the reported dose-response relationships and information on the analytic performance. Only relevant (marine) data that met high quality standards were used in the database. Procedures for risk management were also included. A broad range of organisms and endpoints were assessed, but if insufficient data for the marine environment were available, results from freshwater studies were used. Quality screening for freshwater studies was more limited than for the saltwater studies because the high number of freshwater data did not allow such a high detail level within the framework of the current project. Thus, freshwater data were given a quality score ('reliable', 'reliable with restrictions' or 'not fully verifiable') depending on the data source (e.g. data from EU risk assessment reports are classified as reliable whereas data from the US-EPA ECOTOX database are considered not fully verifiable).

Phase 4: Development of an integrated database with a graphical user interface and modelling of the ecotoxicological data

In the fourth phase the relational database with a graphical user interface was developed. Data were stored in a relational Access database (see Figs 2 and 3). The advantages of using a relational database over typical archive techniques are the powerful querying capabilities, ease for importing and exporting data in a variety of formats, and faster access to data. The database is made accessible to all end-users (experts and non-experts) as a fully web-enabled searching database using a simple graphical user interface and is retrievable via the project website (<http://www.vliz.be/projects/dimas>). In case of accidental spills, all end-users, public services, media and the general public will be able to easily gather objective, quality-assured information.

Information that was entered in the database includes physico-chemical characteristics of the compounds (physical state, melting point, boiling point, density, solubility, vapour pressure, log Kow, ...), acute and chronic ecotoxicological data on different marine and freshwater species, risk and safety phases and GESAMP hazard profiles.

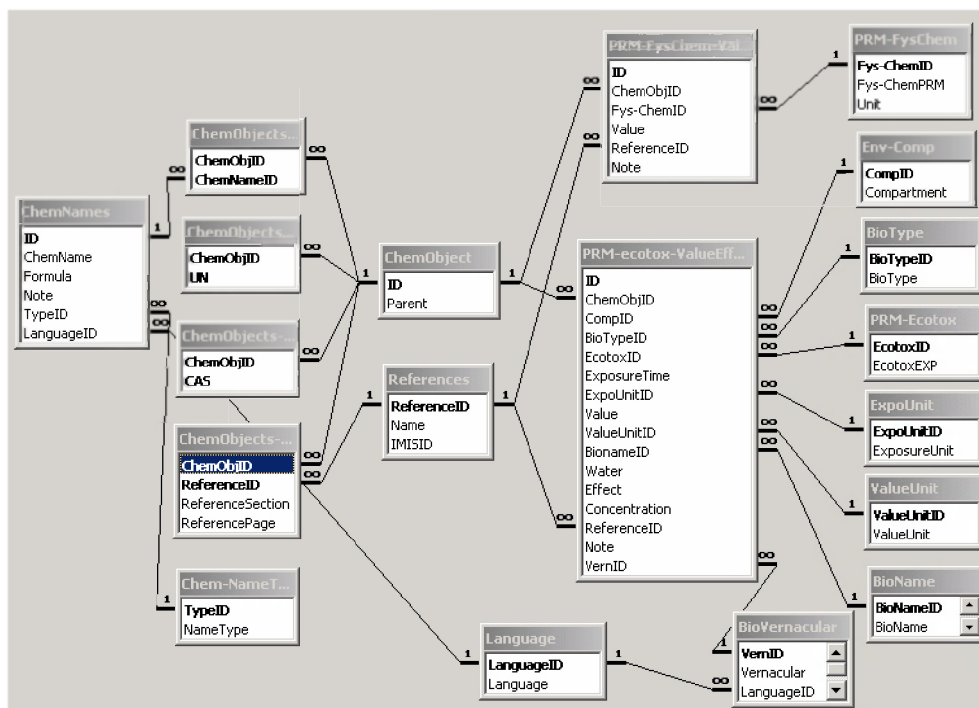


Fig. 2. Structure of the DIMAS database in Access.

The screenshot shows the DIMAS database application interface. The main window displays various data entry fields and a record list:

- ChemObjID**: Formula (C16H22O4), CAS (84-74-2), Parent Object (dropdown), Data Quality (High).
- Note/reason for inclusion**: Text field.
- Species/Other**: Danio rerio (dropdown), Water type (Salt/Fresh), Add or edit species and/or vernaculars.
- Ecotox Exposure Type**: Acute toxicity (dropdown), Compartment (Water), BioType (Fish).
- Values**:
 - Exposure time: 96 (hours), Unit: hour(s).
 - Value: 2.2 (mg/L), Unit: mg/L, Effect concentration: LC50, Analytics: (dropdown).
 - Endpoint: Mortality.
 - Reference: (RAR dibutyl phthalate).
 - Note: (text field).
- Record list**: Shows 1 record of 34 total records.

Fig. 3. DIMAS database in Access.

Based on the amount of the compound spilled and the physico-chemical properties of the compound, the water- or sediment concentration after an accidental spill is estimated (exposure modelling). To facilitate interpretation of the toxicity data, all relevant effect data for a given compound are modelled and visualized in PAF-curves (Potentially Affected Fraction) or

compiled in a Predicted No Effect Concentration (PNEC). An example of a PAF-curve is given in Fig. 4. This curve allows an estimate of the % species that would be affected at a certain environmental concentration and can be calculated for acute and chronic data.

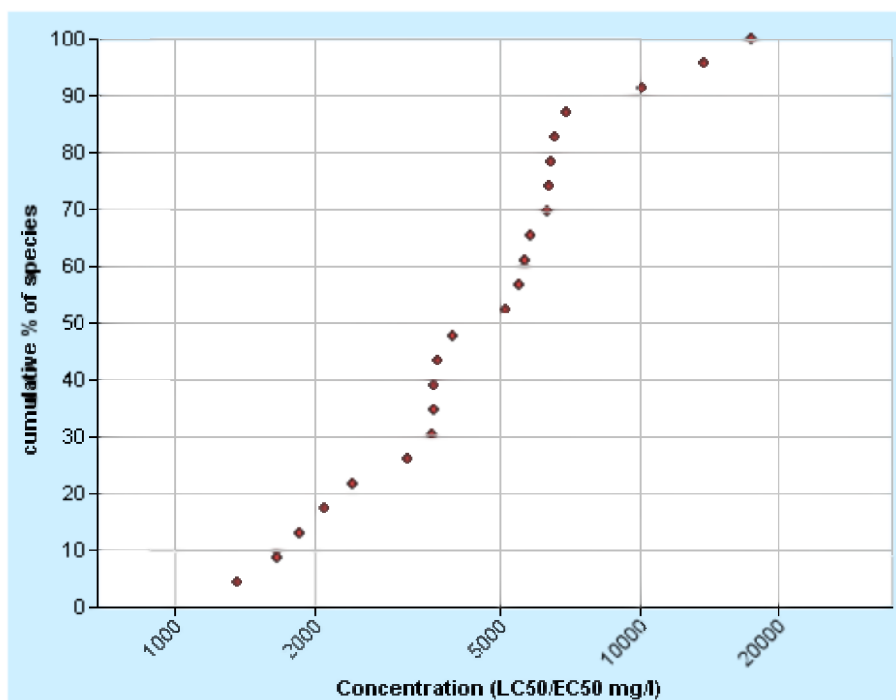


Fig. 4. PAF curve for acute effects acetonitrile (acute LC_{50} or EC_{50} plotted against the cumulative % of species).

The last step in the modelling part of the DIMAS project, was the environmental partitioning modelling. It is very important to estimate which of the compartments (water, sediment, air, biota or soil) is most affected by a chemical spill. This can be done by modelling the behaviour of the compound in the environment. For this purpose, the approach developed by Mackay *et al.* (1996abc) was integrated in the DIMAS database.

Mackay *et al.* (1996abc) describe a multimedia equilibrium criterion model (fugacity model), which can be used to evaluate the environmental fate of a variety of chemicals. The model treats chemicals that fall into three categories. In the first category the chemicals may partition into all environmental media, in the second they are involatile, and in the third they are insoluble in water. The model consists of level I, II, and III calculations. By sequentially doing level I, II and III calculations, increasing information is obtained about the chemical's partitioning, its susceptibility to transformation and transport, and the environmental process and the chemical characteristics that most influence chemical fate. Level I estimates the equilibrium partitioning of a quantity of organic chemical between the homogeneous environmental media with defined volumes, densities, organic carbon contents, and lipid fraction. There are no in- or out-flows of chemical, and no degrading reactions occur. Level II is similar to the Level I described above, but is a steady state model with a constant input rate, rather than single dose of chemical. There is both advective in- and out-flow of chemical from the unit world. Chemical losses can also occur through degrading reactions. Level III does not assume an equilibrium state, but only steady state. The program uses conventional expressions and typical parameters for intermedia transfer by processes such as wet deposition from the air, sediment deposition in the water, and soil runoff. However, for the DIMAS database, only level I calculations are performed as these require the least input information. Output data give

a picture of the chemical's fate in an evaluative or generic environment. For DIMAS, the standard environment was adapted, by virtually eliminating the soil compartment.

For each of the compounds in the database, environmental partitioning can be modelled if enough input data is available (molecular weight, water solubility, vapour pressure, melting point, log Kow). The output of the environmental fate modelling is a partitioning of the compound between air, aerosols, water, sediment, suspended sediments, and biota (fish).

Dissemination

Active dissemination of the compiled information is of key importance for increasing public awareness and understanding by all stakeholders. This is done through a variety of means, e.g. publication of reports and through a project and cluster website, but the true valorisation of the results consists in the use of the integrated and multi-disciplinary database embedded in a fully web-enabled searching graphical user interface (<http://www.vliz.be/projects/dimas>). Data accessibility is improved by using standard formats simplifying data retrieval and use. As such the tool will increase transparency and allow for rapid communication. Furthermore, the output compatibility with already existing impact models was taken into consideration. The first beneficiaries of this tool are the people directly involved in the first phase of a contingency plan for an accidental spill. As such, initial decision making will be facilitated, for example when concerning the level to which the organization should be alerted or mobilized, whether action is required etc. The final indirect beneficiaries are the general public (scientists, journalists, general public, etc.) who will be better informed about the potential impact to man and the environment and ultimately better protected.