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Environmental Exposure Assessment

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ECETOC

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European Centre for Ecotoxicology
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ENVIRONMENTAL EXPOSURE ASSESSMENT

CONTENTS

SUMMARY

In ECETOC Technical Report No. 51 (ECETOC, 1993) a process for the Environmental Risk Assessment of Substances was described which is applicable to all substances, whether new or existing, and to all environmental compartments. The scheme generally follows a stepwise approach in which, if necessary, increasingly refined estimates of the Predicted Environmental Concentrations (PECs) and the Predicted No-Effect Concentrations (PNECs) can be compared in stages.

A number of steps in the overall process could at the time not be described in detail. The main objective of the work presented in this report was to provide more detailed information on how to perform an assessment of environmental exposure on a regional and on a local scale.

Mathematical distribution and fate models are required in the screening and confirmatory phases of environmental exposure assessment. Sensitivity analyses and a critical review of parameters have shown that regional generic fugacity models of the "Mackay level III" type are, in principle, a suitable tool for performing risk characterisation on a regional scale. The model used and partly described in this report is HAZCHEM; the full description can be found in ECETOC (1994b). Such models can be used to point at environmental compartments of concern in a qualitative manner. For chemicals mainly released via diffuse sources, they may also be used quantitatively, provided that the amounts emitted into the environment can be estimated with a sufficient degree of accuracy. The model published by Mackay *et al* (1992) was used as a basis and was adapted to represent a generic European geographic scenario.

To calculate environmental concentrations in local scenarios, approaches for the water, soil and air compartments are proposed. For the water compartment the discharge (direct or via a WWTP) into a river can adequately be modelled with RIVMODEL which is included in the HAZCHEM package. Two scenarios have been proposed, a lowland river scenario with low flow rate and a mountain area river scenario with higher flow rate. A scenario for local air and soil modelling is presented which includes the most relevant exposure routes. Details on indirect human exposure are given in ECETOC (1994a).

Reliable data on release and emission of a substance are the key elements for the calculation of realistic PECs for the different environmental compartments. In the majority of cases release of a substance is determined by the process involved including dedicated treatment and not by the physico-chemical data of the substance. Emission estimation requires scenarios which cover

release, elimination and dilution processes. As could be demonstrated for e.g. chemical intermediates, it is important to use process-oriented release data, to consider all dilution processes (internal and external) and to use reliable elimination data e.g. in a biological waste water treatment plant. For emission scenarios default values for process data, elimination and dilution should be given which cover an average (generic) situation and which can be overwritten when substance-specific data are available. Using only worst case data would lead to unrealistically high PECs.

Furthermore, for the calculation of PECs information on the kinetics of primary biodegradation (degradation of the parent compound) is needed. It is difficult or almost impossible to derive kinetic biodegradation data directly from simple screening tests on ready biodegradation as they are normally available at base set level of the notification of new chemicals. Since ready biodegradation tests are based on the measurement of ultimate biodegradation, no direct correlation between the results from these tests and primary biodegradation exists. Therefore - as a first step - default half-life times/rate constants have to be assigned to substances according to the results obtained in screening tests.

For the prediction of biodegradation rates in the waste water treatment plant a tiered approach including three steps is proposed, whereby steps 2 and 3 are required only if the PEC needs to be refined. At the screening phase a default rate constant of 3 h^{-1} can be assigned to ready biodegradable compounds and to those which reached the corresponding pass level after acclimatisation. At the confirmatory phase rate constants should be directly determined from measurement of primary biodegradation or based on respirometric methods whereas at the investigative phase comparative measurements of influent and effluent concentrations replace the use of default values or calculated rate constants.

An attempt was made to derive biodegradation half-life times for surface waters and soil by evaluating a biodegradation database and industry biodegradation data but due to the limitations of the available data no recommendations on scientifically based default values to be used at screening level could be given although the data suggest that the default values used within existing risk assessment schemes may be overly conservative. At the confirmatory phase the biodegradation rates in soil and surface waters will have to be derived from primary biodegradation testing requiring specific analytical methods or radiolabelled materials. For soil, standard simulation tests are available.

SECTION 1. INTRODUCTION

In environmental exposure assessment the concentration of a substance in the different environmental compartments is estimated based on physico-chemical properties, the production and emission processes, the use and disposal patterns and the properties of the environmental compartments. The 'Predicted Environmental Concentration' (PEC) can therefore be calculated based on knowledge of the quantity of the substance that will enter the environment and the distribution and degradation processes occurring in the environment using generic, representative model environments.

An alternative to such calculations is measuring (monitoring) the environmental concentrations in the relevant environmental compartments according to a pre-planned sampling strategy. This is only possible for substances which are released in quantities large enough to be detectable by appropriate analytical methods after dilution in the environment. In those cases where reliable high quality monitoring data are available, they should take precedence over the predicted PECs.

In ECETOC (1993) a number of steps in the overall process could at the time not be described in detail. Based on the recommendations of this report, a Task Force was established with the following Terms of Reference:

- verify and if necessary refine the ECETOC risk assessment scheme and use product "Release Scenarios" as input for the scheme by applying them to selected well-documented representative substances;

- define generic regional and local environments and recommend mathematical models for the prediction of realistic worst case exposure levels in the environmental compartments of concern;

- recommend approaches for deriving the kinetic constants required for the application of models for the simulation of (bio)degradation in all the relevant environmental compartments and in waste water treatment plants from available test results and verify waste water treatment plant models;

- seek collaboration with the regulatory authorities for the development of a transparent and consistent computerised mathematical model in line with current and evolving guidelines for environmental risk assessment.

In relation to these Terms of Reference, in this report special attention is given to:

- environmental exposure assessment in the context of risk assessment;
- data requirements and the applicability of generic local and regional models;
- release scenarios including background information;
- (bio)degradation kinetics;
- a number of examples for a local and a regional scale.

This report deals with the environmental exposure assessment whereas the exposure assessment for man as a consumer or to substances released to the environment is described in ECETOC Technical Report No. 58 (ECETOC, 1994a).

The purpose of this report is to present the current "state of the art" knowledge on the above topics supplementing the definitions and processes as described by ECETOC (1993), aiming at the development of scientifically based, pragmatic approaches for environmental exposure assessment for both "existing" and "new" substances.

As in ECETOC (1993) most emphasis is placed on the aquatic environment which is generally regarded as the main compartment at risk.

SECTION 2. BACKGROUND

2.1 LEGISLATION

On 30th April 1992 the European Council adopted the "7th Amendment" of Directive 67/548/EEC (EEC, 1992), which came into force on 31th October 1993. Article 3.2 of this Council Directive requires that risk assessment for notified new substances be carried out according to principles laid down in Commission Directive 93/67/EEC (EEC, 1993a) which came into force 20 July 1993.

In the Council Regulation 793/93/EEC on the evaluation and control of risks of existing substances, which came into force 4th June 1993, a risk assessment is required according to Article 10(4) (EEC, 1993b). It will be amended by a Commission Regulation describing the principles of the assessment of risks to man and the environment of existing substances (EEC, 1993c).

Additionally several national authorities and international organisations have developed hazard and risk assessment concepts for new and/or existing substances (e.g. Germany, The Netherlands, UK, Switzerland, USA and the OECD), as documented by ECETOC (1993).

2.2 EXISTING HAZARD ASSESSMENT SCHEMES

In 1990, the Commission of the European Communities, Directorate General XI, organised a workshop on "Environmental Hazard and Risk Assessment in the Context of Directive 79/831/EEC" (EEC, 1990) in collaboration with the Environmental Institute of the Joint Research Centre Ispra. This workshop discussed and identified common principles for the environmental risk assessment of substances to achieve a harmonised and transparent procedure for the evaluation of new substances within the Community.

At the request of the Commission the conclusions of the "Ispra workshop" were discussed by various interested organisations. ECETOC (1991) concluded that the outcome of the Ispra workshop formed a good basis for further discussions. The main points of agreement were that the hazard assessment process should be iterative, that exposure scenarios should be developed for "use-categories" (surfactants, dye-stuffs, solvents, etc.) and that there was a need for differentiation in the assessment process between the exposure from limited point sources and exposure from diffuse release.

The Dutch National Institute of Public Health and Environmental Protection (RIVM) has developed on behalf of the Netherlands Ministry of Housing, Spatial Planning and the Environment (VROM) and the Ministry of Welfare, Health and Cultural Affairs (WVC) a risk assessment software package USES (Uniform System for the Evaluation of Substances) which integrates DRANC (Dutch Risk Assessment New Chemicals), PRISEC (Priority Setting Existing Chemicals) and ESPE (Evaluation System Pesticides) (RIVM, VROM, WVC, 1994; see also Vermeire *et al*, 1992). It is the intention of both DG XI, the Dutch competent authorities and industry representatives to investigate the possibilities of the development of a similar system suitable for performing risk assessments in accordance with the Technical Guidance Documents adopted for notified new substances in 1993 and the Technical Guidance Documents for existing substances (in preparation during 1994).

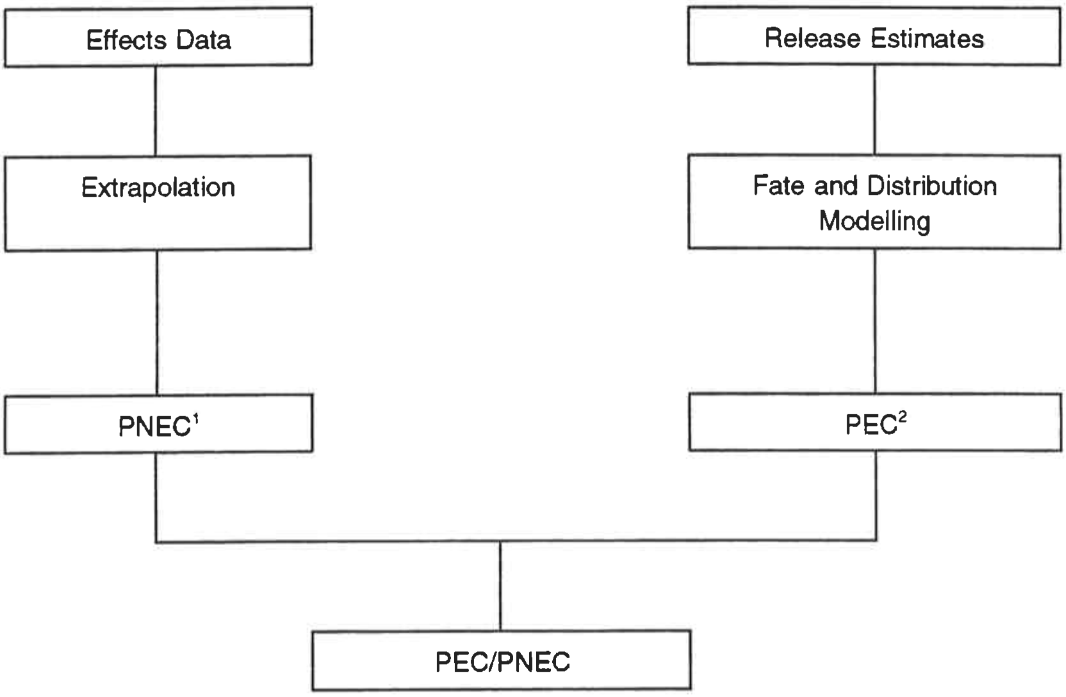
The EU has adopted the Technical Guidance documents for the risk assessment for notified new substances. At the request of DG XI, the German authorities are producing the Technical Guidance documents for the risk assessment for existing substances. Furthermore the UK Government together with UK industries have produced a risk assessment scheme for existing substances (UK, 1993) in the context of EC and OECD existing chemicals programmes.

The existing schemes for risk assessment as developed for new and existing substances by the EC DG XI, generally follow a stepwise approach in which, if necessary, increasingly refined estimates of the Predicted Environmental Concentrations (PECs) and the predicted No-Effect Concentrations (PNECs) can be compared in stages. The necessity of refinement of either PEC(s) and/or PNEC(s), when one of the PEC/PNEC ratios is greater than 1, is based on the assumption that such refinement significantly will reduce the PEC/PNEC ratios to values below 1. If it is obvious that this cannot be achieved, further refinement of either PEC or PNEC is not useful and hence should not be performed.

SECTION 3. ENVIRONMENTAL EXPOSURE ASSESSMENT IN RELATION TO RISK ASSESSMENT

The process of environmental risk assessment was defined and described in ECETOC Technical Report No. 51 (ECETOC, 1993). It was related to production, distribution, use and disposal of substances on a localised scale as well as on a more widespread, 'regional' scale. The risk assessment procedure involves comparison of the PEC of the substance with the best estimate of the concentration which causes no effect to the organisms resident in the environmental compartment of concern (PNEC) (see Figure 1).

Figure 1 Basic Elements of the Hazard Assessment Scheme Resulting in PEC/PNEC Comparisons



1 PNEC = Predicted No-Effect Concentration
2 PEC = Predicted Environmental Concentration

The process therefore includes the derivation of:

- predicted (or measured) environmental concentrations (i.e. exposure assessment);
- predicted no-effect concentrations in the environment (i.e. effects assessment).

It is important to take the PEC and the PNEC into account in a risk assessment, although for the process it is necessary to differentiate between fate (e.g. degradation/persistence) and effects (e.g. acute or chronic toxicity) of the substance. The risk assessment should not be based either on environmental concentrations or effects. Quite often persistence, for instance, is regarded as an undesirable property (effect). Strictly speaking it only relates to the fate of a substance in a particular environment. There are many situations in which persistence is seen as a desirable property, e.g. in polymers, paints, varnishes for construction purposes. Therefore, persistence *per se* should not drive the risk assessment, specifically in the absence of adverse effects.

The risk assessment is conducted as an iterative process. The phases of the exposure assessment can be called screening, confirmatory and investigative and are related to the level of detail of the data used. In the effects assessment the phases are characterised by data from acute, chronic or ecosystem tests from which PNECs are derived by using application factors.

The PEC values needed for the above-mentioned risk assessment can be measured or predicted by applying mathematical models (Section 4). Environmental concentrations depend on the total release and its pattern as well as on the distribution and fate of the substance in the environment. Therefore, important aspects of the environmental exposure assessment are the methods to derive or estimate the total release (Section 5) and methods to estimate degradation (fate) in the different environmental compartments (Section 6).

Discontinuous releases should be treated differently from the continuous releases. The result of discontinuous releases lead to time-dependent concentrations in the environment (variable PECs). To compare these PECs with appropriate PNEC values, the latter will have to be derived from either acute or chronic toxicity tests using a different set of application factors to take into account the temporal variation in PEC values. In the absence of proper tests to account for this variation, acute toxicity tests seem to be most appropriate for deriving PNECs.

SECTION 4. GENERIC ENVIRONMENTAL EXPOSURE MODELS

4.1 INTRODUCTION

Computer models are valuable tools for estimating the concentration of substances in different environmental compartments and to predict the chemical fate of a substance. Input parameters for these estimations are the physico-chemical properties of the substance evaluated and the characteristics of the receiving environmental compartment(s). While physico-chemical parameters are inherent properties of the substance, the nature and properties of the environment may vary widely depending on the location. Moreover, even small ecosystems like a tributary are very complex and are difficult to characterise. In order to decrease the complexity inherent to 'real' environments, the use of a 'generic' or 'evaluative' environment with standard properties has been suggested (Baughman and Lassiter, 1978) and developed (Mackay *et al*, 1992).

By using these 'generic' environments the fate of different substances can be compared under standard conditions. Moreover it is easier to evaluate results for a given substance obtained for different locations. However, it is important to understand that the use of 'generic' environments is no attempt to simulate the 'real' environment, but simply a concept to predict the behaviour of the substance under standard conditions. The inherent disadvantage of these 'generic' environments is that the estimations are difficult to validate. Therefore, figures obtained with these models must be used with great care.

4.2 GENERIC REGIONAL MODEL

The regional generic model may be used to determine the 'compartment of concern' and to estimate the background levels of substances that enter the environment via a diffuse release.

As a basis for the regional exposure assessment a generic regional model based on fugacity described by Mackay *et al* (1992) has been used. ECETOC (1993) indicated the usefulness of this model by some initial sensitivity analyses and by a preliminary validation comparing calculated data with data measured in the environment. It was recognized that this exercise was limited and needed to be elaborated. In this section a critical review of the parameters used and more extensive sensitivity analyses are described with the goal of defining an acceptable regional model scenario for the European situation.