Screening Tool for Assessment of Risks as Result of Emissions of Toxic Substances into the North Sea (SCREMOTOX)

Part I: The screening methodology
Part II: Concise user's manual (version 1.00)

March 1996
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Het ontwikkelde instrumentarium

Het ecotoxicologische risico van de emissie van een toxische stof voor zones van de Noordzee wordt in de screeningsmethodiek SCREMOTOX bepaald door beschouwing van de volledige weg, die een stof aflegt. Deze omvat:

1) emissie naar water en atmosfeer;
2) transport en retentie in rivierstroomgebieden;
3) transport en retentie in de atmosfeer; en
4) verspreiding en retentie in zones van de Noordzee.

Belangrijke kenmerken van de methodiek zijn:

- emissies kunnen worden geschat met de USES-methodiek (RIVM, 1994), gebruik makend van globale gegevens over de productie, invoer en uitvoer van een stof; de gebruiker kan ook met eigen methoden en informatie geschatte emissies invoeren;
- aquatische emissies worden gedistribueerd over alle compartimenten in rivierstroomgebieden, atmosferische emissies worden geaggregeerd op landenniveau;
- aquatische vrachten door verschillende grensvlakken in het systeem kunnen worden vervangen door 'gemeten' vrachten;
- verschillende schattingsmethoden worden gebruikt om 'gemeten' vrachten te bepalen, afhankelijk van het aantal metingen en het gedrag van een stof;
- het transport door rivierstroomgebieden wordt beschreven met 'steady-state' modellen voor compartimenten (2 drainagegebieden, 2 riviersegmenten en het estuarium);
- atmosferische depositie op de Noordzee wordt bepaald voor zones, waarbij rekening wordt gehouden met de aard van de stof en de afstand tussen landen en zones;
- de verspreiding in de Noordzee wordt beschreven met behulp van een 'steady-state' versie van het DELWAQ 4 waterkwaliteitsmodel op basis van het GENO-grid en 'steady-state' hydrodynamische berekeningen met WAQUA (DELT HYDRAULICS, 1994a; Waterloopkundig Laboratorium, 1995b);
- de expositieconcentraties in de Noordzee worden geaggregeerd per zone;
- het ecotoxicologische risico wordt berekend als de verhouding van de waarschijnlijke omgevingsconcentratie (PEC) in een zone en bepaalde effectconcentraties (NEC, EC50); de resultaten worden gerangschikt naar zones en seizoenen;
- aan het voor een stof berekende risico wordt een klasse toegekend, hetgeen de rangschikking van stoffen naar potentieel risico mogelijk maakt;
- natuurlijke variabiliteit wordt beschouwd als de waarschijnlijkheidsverdeling van concentraties binnen een zone, samenhangend met inhomogeniteit en fluctuerende 'forcing' functies; variabiliteit wordt gekwantificeerd op basis van de verdeling gerelateerd aan dispersie; fluctuatie van 'forcing' functies wordt verwaarloosd;
- berekeningen kunnen worden uitgevoerd voor een of meer seizoenen;
- onzekerheid wordt in beschouwing genomen voor zover deze de waarden van stofeigenschappen betreft; andere bronnen van onzekerheid zoals emissies en de intrinsieke onzekerheid van modellen worden om praktische redenen verwaarloosd;
- de invoer voor de methodiek moet zo worden gekozen, dat met het oog op variabiliteit en onzekerheid voldaan wordt aan een 'worst-case' benadering.
De programmatuur van SCREMOTOX bestaat uit vijf modules, die aangestuurd worden vanuit een gebruikersschil. De schil stelt de gebruiker in staat de invoer voor SCREMOTOX samen te stellen en berekeningen uit te voeren op basis van een vraag-en-antwoord benadering. De berekeningen worden onderbroken op verschillende plaatsen om het de gebruiker mogelijk te maken ze te herstarten of te beëindigen, afhankelijk van te verwachten risico’s of tussenresultaten. De schil verschafte informatie met betrekking tot continuering van de berekeningen of de bepaling van invoergegevens. De vijf modules betreffen:

- invoer van ‘case’ informatie, stofeigenschappen, eigenschappen van rivierstroomgebieden, en emissie-gerelateerde gegevens;
- berekening van emissies en atmosferische depositie;
- transport en retentie in de rivierstroomgebieden;
- verspreiding en retentie in de Noordzee;
- uitvoer van expositieconcentraties, concentratieverdelingen, onzekerheidsbanden, bijdragen van de bronnen van emissie aan de totale belasting, en natuurlijk risico’s.

Deel 1 van dit rapport beschrijft de methodiek met betrekking tot gebruiksdoelen, uitgangspunten, ruimtelijke schematisatie, formuleringen, invoer, uitvoer, wijze van omgaan met onzekerheid en natuurlijke variabiliteit. Deel 2 bevat een beknopte gebruikershandleiding.

Conclusies en aanbevelingen

In aanvulling op algemene screeningsmethoden zoals USES (RIVM, 1994) en IPS (RIVM, 1993) is SCREMOTOX specifiek ontwikkeld voor de evaluatie van ecotoxicologische risico’s voor de Noordzee. SCREMOTOX onderscheidt transport en retentie in riviersystemen, estuaria en mengzones van de Noordzee in tegenstelling tot USES en IPS, die niet zijn gebaseerd op geografische schematisatie. De methodiek maakt het mogelijk stoffen te rangschikken naar risico’s en prioriteiten te bepalen ten aanzien van beleidsvorming, monitoring en onderzoek.

De huidige versie van SCREMOTOX is een in technisch opzicht volledig werkend instrument, dat in grote mate voldoet aan het methodologisch ontwerp (Waterloopkundig Laboratorium et al., 1995). Naast noodzakelijk gebleken uitbreidingen moesten vanwege de beschikbare middelen ook beperkingen worden aangebracht. Om tot een direct inzetbaar instrumentarium te komen moeten nog de volgende stappen worden gezet:

- voorzien van SCREMOTOX van realistische en accurate waarden voor de fysische parameters en waterkwaliteitsparameters van de rivierstroomgebieden; en
- validatie van de methodiek voor een tweetal voldoende verschillende ‘cases’.

Aanbevolen wordt om aanvullend de volgende stappen te zetten om een volwaardig en optimaal bruikbaar instrument beschikbaar te maken:

- proefondervindelijke beoordeling van functionaliteit en gebruiksvriendelijkheid door een groep van gebruikers en uitvoering van noodzakelijk geachte aanpassingen;
- verdere uitwerking van de emissiemondeule en opname van de tabellen met emissiefactoren in de programmatuur;
- zonodig detaillering van de formuleringen voor transport en retentie in estuaria;
- vervanging van het jaargemiddelde stroomveld voor de Noordzee door seizoensgemiddelde stroomvelden;
aanbrengen van systematisch onderscheid naar de diverse vormen van natte en droge atmosferische depositie; verbetering van de betreffende formuleringen; vergroting van inzicht in de onzekerheid bij de bepaling van atmosferische depositie;

- opname van methodieken voor normering van concentraties in sediment;

- uitbreiding van de bepalingsmethodieken voor NEC's met QSAR's; opname van de methodieken in de programmatuur;

- uitbreiding van de functionaliteit ten aanzien van kwantificering van bronnen van onzekerheid en natuurlijke variabiliteit, afbreken van berekeningen, aansluiting op data-bases, prioritering voor gegevensverzameling en analyse voor groepen stoffen;

- verbetering van de 'performance' van de programmatuur in een windows-omgeving ten aanzien van ondersteuning van de gebruiker en ten aanzien van rangschikking, grafische presentatie en afdrukken van de uitvoer.

**Beleidsrelevantie**

De ontwikkeling van SCREMOTOX sluit in het bijzonder aan bij de volgende door BEON geformuleerde beleidsvragen:

- Wat zijn de effecten van 'onbekende' stoffen? Hoe kan bepaald worden welke dienen te worden gereguleerd? Aan welke stoffen dient prioriteit te worden gegeven?

- Tot welk niveau moet de concentratie in het veld dalen om negatieve effecten te voorkomen? Wat is de milieugebruikersruimte van stoffen? Zijn er speciale gebieden waar in de toekomst de aandacht op gericht dient te worden?

- Tot welk niveau moet de vraag dalen om negatieve effecten te voorkomen? Wat zijn de belangrijkste bronnen van microverontreinigingen? Hoe groot zijn de atmosferische depositie en lozingen van microverontreinigingen op de Noordzee?

- Wat is de relatie tussen de input van een stof en de concentratie in het sediment en organismen en de mogelijke effecten?

- Welk beleidsanalytisch instrumentarium is benodigd om een beoordeling te kunnen maken van microverontreinigingen?

- Welke monitorsstrategie is noodzakelijk om trends aan te tonen in de concentratie en effecten van microverontreinigingen?

Op al deze vragen kunnen door toepassing van SCREMOTOX antwoorden worden verkregen. Toepassingen kunnen daardoor een bijdrage leveren aan de koppeling van bronigericht en effectgericht beleid. De methodiek kan niet alleen een bruikbaar instrument zijn voor nationale doeelindien, maar ook voor het toestandbrengen van ontwikkelingen in het kader van OSPARCOM en de Noordzeeconferenties.

**Plaats in het BEON-programma**

De ontwikkeling van SCREMOTOX speelde zich af binnen het speerpunt microverontreinigingen. Het project kan gezien worden als directe invulling van het als prioritaar aangegeven onderzoeksonderwerp "Onderzoek naar de effecten van onbekende stoffen". Tevens kan het bijdragen aan het prioritaire onderzoeksonderwerp "Onderzoek naar de atmosferische depositie van microverontreinigingen". Het project richtte zich niet op het opvullen van kennisleemten, omdat het methodiekontwikkeling betreft. Door gebruik van de methodiek zal het echter mogelijk zijn om gerichter te werken aan het opvullen van kennisleemten omtrent de eigenschappen, de emissie, de verspreiding en de effecten van specifieke stoffen.
Summary

In addition to general screening methods as USES (RIVM, 1994) and IPS (RIVM, 1993) the screening methodology SCREMOTOX has been developed for the evaluation of ecotoxicological risks of the emissions of toxic substances into the North Sea. Whereas USES and IPS are not based on any geographical schematization, SCREMOTOX is North Sea specific taking into account transport and retention within river systems, estuaries and North Sea mixing zones. The methodology allows the ranking of substances according to risks and the determination of priorities with respect to policy making, monitoring and research. Besides national application the methodology may be a useful instrument in furthering developments within the framework of OSPARCOM and the North Sea Conferences.

The risk for zones of the North Sea is evaluated in SCREMOTOX considering the whole path of toxic substances. This includes:

1) emission into water and atmosphere;
2) transport and retention in riverbasins;
3) transport and retention in the atmosphere; and
4) distribution and retention in North Sea zones.

Important features of the methodology are:

- emissions may be estimated with the USES-methodology using few input data on production, import and export of the substance, or by the user himself on the basis of his own method and more specific information;
- aquatic emissions are distributed over all aquatic compartments in riverbasins, atmospheric emissions are aggregated in countries;
- aquatic loads at several interfaces of the system may be replaced by 'observed' loads;
- several estimation methods are used to quantify observed loads, depending on the number of available observations and on the behaviour of the substance;
- the transport through riverbasins is described by steady-state box models for two drainage areas, two river sections and the estuary;
- the atmospheric deposition on the North Sea is determined for North Sea zones, taking into account the nature of the substance and the distance between countries and North Sea zones;
- the distribution in the North Sea is described with a steady-state version of the DELWAQ 4 water quality model on the basis of the GENO-grid and steady-state hydrodynamic calculations with WAQUA (DELFt HYDRAULICS, 1994a; Waterloop-kundig Laboratorium, 1995b);
- the exposure concentrations in the North Sea are aggregated in zones;
- the ecotoxicological risk is calculated as the ratio of the probable environmental concentration (PEC) in a zone and certain effect concentrations (NEC, EC₉₀); the results are ranked according to zones and seasons;
- one of four risk classes is attributed to the risk computed for a substance, which allows the ranking of substances;
natural variability is considered as the probability distribution of concentrations in a zone resulting from inhomogeneity and fluctuating forcing functions in the natural system; the variability is quantified on the basis of the concentration distribution within a zone connected with dispersion; the fluctuation of forcing functions is ignored;

- computations can be performed for one or more seasons;
- uncertainty is taken into account regarding the uncertainty of parameter values for substance characteristics; other sources of uncertainty such as emissions and the intrinsic uncertainty of models are ignored for practical reasons;
- the input to the methodology is to be selected taking sources of variability and uncertainty into account in such a way that a worst case approach is obeyed.

The SCREMOTOX-software consists of five FORTRAN-modules, operated through a user interface. The REXX-based interface program allows the user to compose the input for SCREMOTOX and to run its computational parts on the basis of a question-decision procedure. The computations are interrupted at several stages in order the enable the user to restart or to terminate the session depending on expected risks or intermediate results. The interface also provides information regarding continuation of the computations and regarding the determination of input data. The modules operated from the user interface concern:

- input of case information, substance characteristics, river basin properties and emission-related data;
- computation of emissions and atmospheric deposition;
- transport and retention in the riverbasins;
- distribution and retention in the North Sea;
- output of exposure concentrations, concentration distributions, uncertainty ranges, contributions of emission sources to the total load, and of course risks.

Part 1 of this report describes the methodology in terms of objectives, starting points, spatial schematization, formulations, input, output and dealing with uncertainty and natural variability. A concise user’s manual focusing on the user interface is presented as part 2.
Introduction

Background

In addition to general screening methods as USES (RIVM, 1994) and IPS (RIVM, 1993) the screening methodology SCREMOTOX has been developed for the evaluation of ecotoxicological risks of the emissions of toxic substances into the North Sea. Whereas USES and IPS are not based on any geographical schematization, SCREMOTOX is North Sea specific taking into account transport and retention within river systems, estuaries and North Sea mixing zones. The methodology allows the ranking of substances according to risks and the determination of priorities with respect to policy making, monitoring and research. Besides national application the methodology may be a useful instrument in furthering developments within the framework of OSPARCOM and the North Sea Conferences.

The task of developing SCREMOTOX was commissioned by BEON in March 1995 to Delft Hydraulics as principal contractor and to TNO-MW. These institutes carried out the project in co-operation with the National Institute for Coastal and Marine Management (RIKZ, Rijkswaterstaat, Ministry of Public Works) and the National Institute for Public Health and Environmental Protection (RIVM). Contributions were also delivered by the National Institute for Inland Water Management and Waste Water Treatment (RIZA, Rijkswaterstaat, Ministry of Public Works) and the Directorate General for Environmental Protection of the Ministry of Housing, Physical Planning and Environment (DGM).

Project outline

The project was carried out in two phases. Phase one yielded the methodological design of SCREMOTOX, basically a description of the functions, the structure, the main formulations, the input and the output (WL et al., July 1995). The fundamentals of the design were laid down during a workshop, into which RIKZ, RIVM, DGM, RIZA, TNO-MW and WL participated. Further elaboration of the design and the actual development of the tool, including the building of the computer programme, took place in phase two.

Special attention was paid to the question-decision procedure, through which the user communicates with SCREMOTOX. The procedure informs the user on options to choose from and on steps to be taken. The procedures aim to establish a minimum of undefined uncertainty in the results of the computations. Computations may be interrupted or terminated at the point were continuation is no longer meaningful. This may be the case when inaccuracy or uncertainty becomes too large or when the expected risk is insignificant. The outcome of the computations for individual substances allow ranking of the substances according to risks.
Development stage

The design of the screening methodology is ambitious. The available budget did not permit full realization of the specifications of the design. However, it is thought that the present version of SCREMOTOX allows successful application for risk assessment and ranking of substances, provided that the tool be filled with appropriate data for the physical system characteristics of the riverbasins discharging into the North Sea. Improvements are expected with respect to the question-decision procedure and the user interface, especially regarding the presentation and reporting of output.

The report

The report consists of two parts. Part 1 describes the methodology. This includes the definition of SCREMOTOX, its functionality, the formulations and specification of input and output. The sections on formulations deal with emission, transport and retention in surface water, transport and retention in the atmosphere, partitioning and exposure, and ecotoxicological risk.

Part 2 contains a concise user manual, which focuses on the user interface. Moreover, specifications are given with respect to hardware and software.

Project execution


The computer application of SCREMOTOX was constructed and programmed by J.G. Boon and R. van Buren (WL).

The report was written and composed by J.G.C. Smits, using contributions of:

- J. Knoop; emission
- T. Smit; use of observed concentrations for load determination
- J.G. Boon; distribution modelling for the North Sea
- A.C. Baart; atmospheric deposition
- H.P.M. Schobben; ecotoxicological risk assessment
- H.G. Evers; input of substance characteristics
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1 Tool definition

The tool for screening of substances with respect to the ecotoxicological risk for the North Sea arising from emissions of these substances into the environment is a computer programme that allows for:

- quantification of the exposure of organisms in several mixing zones of the North Sea to any toxic substance;
- estimation of the ecotoxicological risk in the zones of the North Sea resulting from the exposure to this substance;
- ranking of substances with respect to their (potential) ecotoxicological risks for the North Sea; and
- assessment of the sources of emission of a toxic substance.

Application of the tool has to support the determination of priorities with respect to policy making, monitoring and research.

The tool is different from general methods as USES and IPS (RIVM, 1993 and 1994) in the sense that it is North Sea specific. It actually considers the river basins, the transportation routes and the mixing zones of the North Sea system. This requires that the retention and distribution factors connected with the various aquatic and atmospheric compartments and with homogeneous subsets of substances are intrinsic properties of the screening tool.

The screening tool describes the whole path of a substance to and through the North Sea. This includes all stages from production to transportation through and retention in surface water and atmosphere. The computer programme of the screening tool therefore has a modular structure. The modules relate to:

- supply of input data through a procedure on basis of a question-decision approach;
- quantification of emissions of a substance into the natural system as the result of production and application;
- quantification of transport and retention of a substance in the natural system, that is drainage systems, river systems, estuaries, North Sea zones and the atmosphere; and
- production of output concerning the exposure of North Sea zones to a substance, the inherent ecotoxicological risk and the emissions.

The modules are linked up with an user interface, that takes care of reading input, communication with the user, execution of maximally four seasonal steady-state computations, and the production of output.
The starting points for the formulation of the screening methodology, including a few definitions, have been as follows:

- Concentrations are defined as probable exposure concentrations (PEC) and have a natural variability distribution and an uncertainty band.
- Risk classes are related to three specific test values, e.g. effect concentrations such as the NEC. The NEC is a measure for the sensitivity of the ecosystem to the presence of toxic substances. Risk is defined as the ratio of the probable exposure concentration and a specific effect concentration, in particular the PEC/NEC-ratio. However, differences of risks for populations or specific organisms are not considered because these differences can not be quantified as yet in terms of effect concentrations.
- Violation of a test value is primarily calculated on the basis of the 95-percentile value of the natural variability distribution of a concentration. Secondarily, the uncertainty interval is taken into account.
- Both concentration and risk are computed as time average values on a seasonal timescale. A full computation may therefore produce different results for each season. The duration of emission (pesticides) is checked against the duration of transportation to and in the North Sea.
- Concentrations and risks for the zones in the North Sea are ranked according to a) magnitude and b) season. The highest seasonal value determines the ranking of the zones.
- The compartments that shape up the aquatic transportation routes from the locality of the emissions to the zones of the North Sea are grouped according to river basins. A river basin encompasses one or more drainage systems, one a more river sections (including tributaries), an estuary and the affected zones in the North Sea.
- Zones in the North Sea are rather well mixed, are rather homogeneous with respect to settling, are a part of the area affected by a river basin, have a specific value as ecosystem or resource, and/or are specifically sensitive to toxic substances. The number of zone has been limited because of practical reasons.
- Transportation through a compartment or zone is determined using compartment specific and substance specific retention factors (sum of loss factors) and distribution factors. The retention factor is defined as the fraction or the percentage of the incoming mass flux that is retained in a compartment, both by storage in the sediment and by decomposition. The distribution factor is defined as the fraction or the percentage of the incoming mass that is transported to another compartment.
- Emissions may be caused by point sources and/or diffuse sources. They may be land based or sea based. The latter are related to the offshore industry, to shipping and to the disposal of waste material, such as dredging sludge. However, all emissions are assumed to be continuous and completely dispersed into a compartment or a zone, which implies that near-field and short term effects of (necessitous) emissions can not be evaluated with the screening tool.
- Sources of emissions into aquatic compartments are subsequently grouped according to countries, riverbasins and compartments.
- The sources of emission into the atmospheric compartment are grouped according to countries.
• Natural variability arises from inhomogeneity and from fluctuating forcing functions in the natural system. Uncertainty adheres not only to substance specific process parameters, emissions and effect concentrations but also to the concept of a simplified steady-state model.

• The natural variability is quantified on the basis of the concentration distribution within a zone connected with dispersion. The fluctuation of forcing functions is ignored.

• The uncertainty in substance specific process parameters is taken into account explicitly. The intrinsic uncertainty of a simplified steady-state model is ignored for practical reasons, as well as the uncertainties in the magnitudes of emissions and effect concentrations. Quantification appears to be very difficult often. This is due to a lack of data or to the laboriousness of the acquisition of data. In stead of considering inaccuracy, one should determine maximal yet realistic estimates of emissions and minimal estimates of effect concentrations. Such a worst case approach is in line with the activity of screening.

• The methodology has been designed for a worst case approach. However, the computation must bear a minimum of (ill-defined) uncertainty. The computed mass fluxes into or between compartments may therefore be replaced at the interfaces of certain compartments with mass fluxes determined on the basis of concentration measurements in rivers or estuaries.

• The synergy of toxic substances is not taken into account explicitly. Ignoring synergy may lead to incorrectly judging of substances as being non-problematic.

The North Sea screening tool is made using building blocks of other screening tools (USES) concerning the production, application and emission of substances. Moreover, physical characteristics required to calculate the retention and distribution factors and the concentrations can be generated from dynamic simulations with existing detailed models describing the fate of micropollutants in the aquatic system or the atmospheric system. This may be done with the following models developed by DELFT HYDRAULICS or TNO (atmospheric model):

• PRELUDE en the PAWN-distribution model for the drainage system;
• DELWAQ/IMPAQT for the river system;
• a series of estuarine retention models (ECOS, simple DELFT HYDRAULICS-model, SAWES);
• SHELF-model for micropollutants for the North Sea; and
• the atmospheric transport and retention model of TNO.
2 Specification of functionality

Specifying the functions of the screening tool starts off with formulation of the management issues. The main relevant questions are:

- Which substances pose a threat to the marine ecosystem of the North Sea?
- Which substances pose the greatest threats?
- Where do the emissions of these substances come from and which are the (dominant) sources?
- How can source oriented policies be strengthened by means of effect oriented policies?
- What are the priorities with respect to policy making (emission control) and data collection (research, monitoring) for toxic substances?

Consequently, the screening tool was made for the assessment of both the absolute and the relative risk of micropollutants. The use of the tool supports the formulation of policies and priorities for both management of the emissions of toxic substances and research concerning their properties. The results produced from applications of the tool may support the coordination between the authorities involved in management and protection of the North Sea, both nationally and internationally (OSPARCOM, North Sea Conferences).

Considering the above, the main function of the screening tool is the computation of:

- the total, dissolved and particulate concentrations of any micropollutant in the water, the sediment and the biota of mixing zones in the North Sea, resulting from the collective sum of emissions in the bordering countries and at sea;
- the total, dissolved and particulate concentrations of a micropollutant in the water and sediment of the main compartments that shape up the aquatic transportation routes from the emissions to the North Sea;
- the ecotoxicological risk of any organic micropollutant in the water and sediment in the zones, resulting from the calculated exposure; and
- the mass fluxes of a micropollutant into and between the compartments, including the atmospheric deposition at the zones of the North Sea.

The computation of the concentrations is performed stepwise, going from land to sea. The computations may be interrupted or terminated, when further computations are unacceptable (insufficient or too uncertain input data) or unnecessary (no risk expected). A worst-case approach must avoid the occurrence of too optimistic results as one of the possible consequences of uncertainty in models and input.
To enhance the usefulness of the screening tool for supporting policy making, the tool provides information on:

- reasons for interruption and termination of the computation;
- the dominant sources of pollution; this requires determination of the relative contributions of the sources to the computed concentrations;
- the uncertainty bands around the computed concentrations connected with the uncertainty of values for properties of substances and the variability of the physical system;
- actions how to deal with uncertainty; and
- assignment of one of several classes to the computed risk, according to which the ranking of substances may be done.

The information is partially provided on the basis of a question-decision procedure, allowing the user to choose from several options at critical points in the computation. The answers given by the programme force the user to think about the optimal continuation of the computation or aborting it. The programme also presents suggestions as to how to proceed the activities on the basis of built-in criteria. Suggestions for the selection and quantification of input data in order to exclude undefined uncertainty as much as possible are provided in a protocol included in the user’s manual of the screening tool.

The above functionality has been partially realized in the present stage of development of SCREMOTOX. Future versions should also provide information on:

- the sources of uncertainty, requiring determination of the relative contributions of the sources of uncertainty and variability; and
- the priorities for data collection (research and monitoring).
3 Description of the methodology

3.1 Emission and loads

SCREMOTOX considers land and sea based emissions next to the transport of a substance across the interfaces of the North Sea and the Atlantic Ocean. The following types of emission are considered:

1. emissions into surface water systems of river basins;
2. atmospheric emissions; and
3. direct emissions into the North Sea.

Type 1 emission leads to riverine loading of the North Sea. Type 2 causes a load through atmospheric deposition. Type 3 is either caused by sources on the North Sea, such as ships and offshore industry, or by sources which are located close to the shore, such as water systems not included in major riverbasins (e.g. Frisian 'Boezem' waters). Figure 3.1 presents the pathways of substances between sources and the North Sea. Indicated in gray is the contribution of the atmospheric deposition to the riverine loading of the North Sea. SCREMOTOX ignores this contribution, as it is often small compared to the total riverine loading of the North Sea. This also implies, that volatilization of a substance from surface water creates a permanent sink in SCREMOTOX. The volatized quantity does not contribute to loading of the North Sea via deposition.

Figure 3.1 Pathways between sources and North Sea (exchange with the Atlantic Ocean not included)

SCREMOTOX has three options to quantify emissions or loads, which may be combined in any fashion to suit the needs of the user. The options are:

- estimation of type 1 and 2 emissions on the basis of the emission module of the evaluation system for existing and new substances USES;
- imposing of prefixed emissions for types 1 and 2 in riverbasins and countries, and for type 3 in North Sea zones; and
- imposing observed concentrations for the estimation of riverine loads.
Basically, emissions are quantified as the product of a production or use quantity and an emission factor. This factor indicates the fraction of mass entering the aquatic system or the atmosphere. The fraction is not only closely connected with the type of production or use, it also depends very much on local:

- production and discharge directives, connected with environmental laws and standards;
- practices, related to the level of education, working methodologies, and physical and social constraints; and
- geographic and hydrological conditions, affecting the drainage system.

USES estimates emissions in European countries, using the HEDSET database of emission factors classified for type of industry and substance properties (RIVM, 1994). Differences between countries are ignored.

A production or use quantity can be available directly, but in many cases it has to be estimated. Such estimations usually rely on parameters regarding gross production, economics and demography. Examples are the amount of a raw material used in production, the size of a sectoral activity (for instance agricultural land use), economic value of produced materials, the amount of a product sold on the internal market, and the size of the population. A systematic approach of all these features at the determination of quantities could not be carried out for the present version of SCREMOTOX. The present methodology assumes that production and use quantities are available.

Section 3.1.1 deals with the USES-estimation methodology. The methodology provides aquatic emissions into riverbasin compartments, the transport and retention of which is described in section 3.2, and atmospheric emissions, the deposition of which is described in section 3.3. The estimation of ‘observed’ riverine loads is described in section 3.1.2.

Inflow across the interfaces of the North Sea with the Atlantic Ocean and the Baltic Sea is taken into account by multiplying a user-specified boundary concentration with a flow rate.

### 3.1.1 The emission module

The emission module is based on four elements:

- the production and/or use of the substance in EC-countries;
- factors to assess the emission per unit of production or use;
- factors to assign the fraction of the total emission of EC-countries to individual countries and river basins on the basis of landuse; and
- chemical properties which determine the emission factors and the retention in sewage water treatment plants (STP).

The estimation is based on combination of the substances life cycle (Figure 3.2), two HEDSET classifications (Appendix A) and two chemical properties: vapour pressure and solubility.
Figure 3.2  Life cycle of substances

The general emission model is based on simple linear equations:

$$E_i = \Sigma(fac_{s,i} \cdot P_{EC,i})$$  \hspace{1cm} (3.1)

in which:
- $fac_{s,i}$ = emission factor for life cycle stage $i$ (tn/tn; F[cat$_i$, cat$_{II}$, Vp, So, $K_{ow}$, $facs_i$(cat$_i$,cat$_{II}$)]
- cat$_i$ = main category (HEDSET)
- cat$_{II}$ = industrial category (HEDSET)
- $E_i$ = total aquatic emission in (sub)basins (g-period$^1$)
- Vp = vapour pressure (Pa)
- So = solubility (mg/l)
- $K_{ow}$ = octanol-water partition coefficient (-)
- $facs_i$ = factor to assign emissions to (sub)basin $s$ (-)
- $P_{EC,i}$ = EC production/use of a substance (tn$/a$
- $s$ = (sub)basin (Scheldt, Meuse, Rhine, Ems, Weser, Elbe,...)
- $l$ = substance life cycle stage (production, formulation, processing, private use, recovery)

For air emissions the same module is used with different emission factors and different factors to assign the emissions to the individual countries.

EC production and use

Most of the North Sea river basins are located in EC countries. Since scarce and often incomplete information on production and use on a country level is available for the major part of the substances, the emission estimation will be based on the production and use in the whole of the EC. The net mass flow within the EC-countries is equal to the sum of production and import minus export. Figure 3.3 shows the relation between the elements of the life cycle and these EC values.
Emission factors

For every life cycle stage emission factors are available in USES/HEDSET. Tables have been compiled in Appendix A in hierarchical order according to:

- main category;
- industrial category;
- solubility; and
  - saturated vapour pressure

Although sometimes a further differentiation is available according to the HEDSET use category or even more detailed, for the sake of simplicity this module will make use of the default values, which are worst case values for the different combinations of industrial and main category. First of all, it requires an expert to classify the production, use and application of a substance with more detail than both first HEDSET categories, and secondly, it is questionable whether this extra refinement is in proportion with other assumption in the whole screening tool or even necessary regarding the goal of the tool.

Sewage treatment plant retention

All releases from the life cycle stage to surface water are assumed to enter a sewage treatment plant with one exception: substances classified to industrial category 1: the agricultural industry (application of agricultural chemicals). This is a rough assumption, since not all industries and inhabitants are connected to a sewage treatment plant. In 1988 about 50% of the EC population was served. Yet, especially the countries around the North Sea form a positive exception with percentages of over 80%. Since then, the situation has improved. The STP-model reads:

\[ E_{\text{effluent}} = E_{\text{effluent}} \cdot (1 - R_{\text{rrp}}) \quad (3.2) \]
The retention factor $R_{ow}$ will simply be determined as a function of the octanol-water partition coefficient ($K_{ow}$) and the constant of Henry, which again is a function of the vapour pressure and the solubility with the use of the STP-model Simpletreat (Struijs et. al., 1991). Results of this model can be summarized in a table with classes of both coefficients.

**Location factors**

For each of the pathways for the various categories, emissions must be assigned to the river basins in each country with the use of general available information like land use and population density, which is closely connected with the specific type of emission. Especially for diffuse sources these variables are very suitable for this purpose. The apportionment of industrial point sources with the use of more general information however can be a source of large errors. Although population density or urban land use are closely related to industrial activities they do not provide any information on the exact location of the industrial sources. Therefore, an option of the emission module is to give the user the opportunity to replace estimations generated with the USES-methodology with own values.

The assignment of the total emission of EC-countries to surface waters in the various river basins is done using the ratio between urban land use in the river basins and in the whole of the EC-countries involved. An exception is made for the assignment of the emission caused by the processing of substances classified to industrial category 1. The agricultural industry (application of agricultural chemicals) will be based on the agricultural land use ratio. For parts of the Elbe and Rhine basin, lying outside the EC (mainly The Czech Republic and Switzerland), the estimation of the emissions is done by simply extrapolating EC-values.

Within a river basin further splitting up of the emission occurs among the drainage areas, that are distinguished. Underestimation of riverine loads due to overestimation of retention in the drainage areas may be the result, especially in case of non-agricultural use of a substance. Such underestimation can be counteracted by the user when assigning ‘prefixed’ emissions to other compartments in a river basin, that is the river sections and the estuary. The prefixed emissions are subtracted from the total estimated aquatic emissions for drainage areas.

The atmospheric emissions are divided among the EC-countries using the same land use types. The emissions of non-EC-countries are also estimated on the basis of extrapolation.

**Time scale**

Ecotoxicological risks are computed as time average values on a seasonal time scale. The USES-methodology delivers emission estimates on a yearly average base. The input for SCREMOTOX concerning the net mass flux must take this difference into account. The following extreme situations are defined to transform the available yearly quantities to seasonal ones, accounting for the worst and the best situation respectively:

1. $E_{season} = E_{year} / 4 \cdot (g \cdot period^{-1})$ in case emission can not be assigned to particular seasons
2. $E_{season} = E_{year}$ in case emission is mainly occurring in one particular season
However, the user may follow his own preference, because the choice regarding the approach affects only the input of SCREMOTOX. He may choose to carry out calculations for both extreme situations and any intermediate condition.

**Formulations**

The aquatic emission in basin $s$ and the atmospheric emission in country $c$ are:

\[ E_{-w_{i}} = \left[ \text{fac}_\text{urban}_{c} \times \left( \sum_{i} (E_{-EC_{-w_{i}}}) - E_{-EC_{-w_{process_{s}}}} \right) \right] \times \left( 1 - R_{np}(H,K_{w}) \right) + \text{fac}_\text{agricult}_{c} \times E_{-EC_{-w_{process_{s}}}} \]

\[ E_{-a_{i}} = \text{fac}_\text{urban}_{c} \times \left( \sum_{i} (E_{-EC_{-a_{i}}}) - E_{-EC_{-a_{process_{s}}}} \right) + \text{fac}_\text{agricult}_{c} \times E_{-EC_{-a_{process_{s}}}} \]

if $\text{cat}_{ij} = 1$ (agricultural industry) and

\[ E_{-w_{i}} = \left[ \text{fac}_\text{urban}_{c} \times \left( \sum_{i} E_{-EC_{-w_{i}}} \right) \right] \times \left( 1 - R_{np}(H,K_{w}) \right) \]

\[ E_{-a_{i}} = \text{fac}_\text{urban}_{c} \times \sum_{i} E_{-EC_{-a_{i}}} \]

(3.3)

for all other industrial categories (see below for explanation of parameters)

The emissions appear as loads $L$ in section 3.2.2. Total emissions per life cycle stage $l$ to surface water $w$ and atmosphere $a$ in EC-countries are:

\[ E_{-EC_{-w_{i}}} = \text{fac}_\text{water}_{c}(\text{cat}_{i,ij},V_{p},S_{o}) \times P_{i} \]

\[ E_{-EC_{-a_{i}}} = \text{fac}_\text{air}_{c}(\text{cat}_{i,ij},V_{p},S_{o}) \times P_{i} \]

(3.5)

Total volumes per life cycle stage $l$ in EC-countries are:

\[ P_{production} = P_{-EC} \]

\[ P_{formulation} = P_{-EC} \]

\[ P_{process_{s}} = P_{-EC} + I_{-EC} - EX_{-EC} \]

\[ P_{private} = (P_{-EC} + I_{-EC} - EX_{-EC}) \times (1 - \sum_{p} E_{process}) \]

\[ P_{recovery} = (P_{-EC} + I_{-EC} - EX_{-EC}) \times (1 - \sum_{p} E_{process}) \times (1 - \sum_{p} E_{private}) \]

(3.6)
in which:

\( P_{EC} \) = production in EC-countries (tn/a)

\( I_{EC} \) = import in EC-countries (tn/a)

\( E_{EC} \) = export out of EC-countries (tn/a)

Total emissions for life cycle stages processing and private use in EC-countries are:

\[
\sum_{r} E_{\text{process}} = \left[ \sum_{r} \text{fac}_{p\text{process}} \left( \text{cat}_{1}, \text{cat}_{II}, \text{Vp}, \text{So} \right) \right] \ast P_{\text{process}}
\]

\[
\sum_{r} E_{\text{private}} = \left[ \sum_{r} \text{fac}_{p\text{private}} \left( \text{cat}_{1}, \text{cat}_{II}, \text{Vp}, \text{So} \right) \right] \ast P_{\text{private}}
\]

(3.7)

Emission factors:

\( \text{fac}_{\text{water}}_l \) = emission factor for water for life cycle stage l (tn/tn)

\( \text{fac}_{\text{air}}_l \) = emission factor for atmosphere for life cycle stage l (tn/tn)

\( \text{fac}_{p,l} \) = sum of the factors for water and air (tn/tn); See Appendix A to determine individual factors for every combination of arguments \( \text{cat}_{1}, \text{cat}_{II}, \text{Vp}, \text{So} \)

\( \text{cat}_{1} \) = main category (HEDSET)

\( \text{cat}_{II} \) = industrial category (HEDSET)

\( \text{Vp} \) = saturised vapour pressure (Pa)

\( \text{So} \) = aqueous solubility (mg/l)

\( l \) = life cycle stage (production, formulation, processing, private use, recovery)

\( p \) = compartment (soil, water, air)

Land use factors are:

\[ \text{fac}_{urban,e} = \frac{\text{total}_{urban}\_\text{land}\_use_e}{\text{total}_{urban}\_\text{land}\_use_{EC}} \]

\[ \text{fac}_{urban,c} = \frac{\text{total}_{urban}\_\text{land}\_use_c}{\text{total}_{urban}\_\text{land}\_use_{EC}} \]

\[ \text{fac}_{agricult,e} = \frac{\text{total}_{agricultural}\_\text{land}\_use_e}{\text{total}_{agricultural}\_\text{land}\_use_{EC}} \]

\[ \text{fac}_{agricult,c} = \frac{\text{total}_{agricultural}\_\text{land}\_use_c}{\text{total}_{agricultural}\_\text{land}\_use_{EC}} \]

(3.8)

in which:

\( s \) = (sub)basin (Scheldt, Meuse, Rhine, Ems, Weser, Elbe, ...)

\( c \) = European country (Albania, Austria, Belgium, Bulgaria, ...)
Values can be derived from the tables in Appendix A for urban and agricultural land use for all European countries, all North Sea river basins, and for the whole of the EC.

The retention of sewage water treatment plants (\( R_{sp} \)) is described with:

\[
R_{sp} = (-0.71 \times H + 98.7) / (1 + 0.5 \times e^{(2 \times K_{ow} - 6)})
\]  

\( H = M_w \times V_p / S_o \)

in which:

- \( H \) = constant of Henry (Pa.m³.mol⁻¹)
- \( K_{ow} \) = octanol-water partition coefficient (l/kg)
- \( M_w \) = molecular weight

The formulation for \( R_{sp} \) was derived by curve-fitting on data provided in Appendix A (Struis et al., 1991).

### 3.1.2 Quantification of observed loads

#### General approach

As previously indicated, the user of SCREMOTOX may replace loads computed from estimated emissions and from retention in drainage areas with 'observed' loads. SCREMOTOX has been provided with an algorithm to quantify these loads using observed concentrations and flow rates. Determination of a riverine load as the product of flow rate and concentration may seem rather straightforward. However, available data will be inaccurate to a certain extent and will almost certainly not cover continuous periods. Due to variations in discharge as well as in concentration, loads estimated for certain period of time may not be representative for a longer period. The load calculated from observations will therefore bear uncertainty, which can be determined as a function of the observation density and the observation period. Such estimation methods are described here. They were derived from work reported by De Vries and Klavers (1994).

Continuous water discharge records are usually available. However, this is not the case for concentration data. In general, these data represent individual samples taken at weekly, biweekly or even greater intervals. Several numerical procedures were used by de Vries and Klavers to estimate loads on the basis of continuous water discharge records and limited concentration data. It turned out that three relatively simple procedures can be used best to quantify loads and the inherent inaccuracy. The inaccuracy intervals as a function of observation frequency have been determined for the following three types of rivers:

- sluice systems;
- mixed rained and glacial rivers, like the Rhine; and
- rained rivers, like the Meuse.
In case of the first type there is no clear relation between flow rate, concentration and load. Moreover, the following three types of substances have been distinguished:

- continuously emitted, conservative dissolved substances like chloride;
- seasonally emitted, non-conservative dissolved substances like ammonia; and
- seasonally discharged conservative particulate matter like suspended matter.

As most micropollutants can be considered conservative relative to the rather short residence times in rivers, it was decided only to consider the chloride- and suspended matter types. A micropollutant is a chloride type substance when more than 50% dissolved, a suspended matter type substance when more than 50% adsorbed onto suspended matter. The load estimation methods used by de Vries and Klavers and the accuracy intervals that they found for Rhine and Meuse have been adopted in SCREMOTOX. It is obvious that other rivers discharging into the North Sea, although comparable to one of these two rivers regarding discharge type, may show a somewhat different behaviour. The accuracy intervals for the rivers Rhine and Meuse must therefore be considered indicative for the other rivers.

**Formulations**

De Vries and Klavers performed the accuracy analysis for annual loads. It is assumed that similar accuracy intervals may be used for mean daily loads. The three methods and connected formulations for quantification of the loads are:

1. The simplified method:

   \[ L = K.Q_m \cdot (\sum_{i=1}^{n} C_i/n) \]  

   (3.10)

2. The direct method:

   \[ L = K \cdot (\sum_{i=1}^{n} (C_i/Q_i/n)) \]  

   (3.11)

3. The weighted concentration method:

   \[ L = K.Q_m \cdot (\sum_{i=1}^{n} (C_i/Q_i)) / (\sum_{i=1}^{n} Q_i) \]  

   (3.12)

   in which:

   - \( n \) = number of samples
   - \( L \) = mean daily load (g.day\(^{-1}\))
   - \( K \) = conversion factor to take account of sampling frequency and units
   - \( C_i \) = average concentration in a combined sample over a 24-hours period (g.m\(^{-3}\))
   - \( Q_i \) = 24-hours discharge at the date of sampling (m\(^3\).day\(^{-1}\))
   - \( Q_m \) = mean annual or seasonal discharge based on daily flow measurements (m\(^3\).day\(^{-1}\))
Monte Carlo computations with these formulations provided 95% confidence intervals of the load probability functions. These intervals are taken as useful accuracy intervals for SCREMOTOX. The intervals are presented in Table 3.1 for methods 2 and 3 as function of the sampling frequency. The intervals are calculated in SCREMOTOX using curve-fitted functions (a.N°)

In general, methods 2 and 3 with intervals 2a and 3a/3b have been found appropriate for mixed (a) and rainfed (b) rivers, respectively for dissolved type substances and particulate type substances. Method 2 is to be used when no daily discharge data are available. Method 1 can be used for sluice type rivers in combination with the accuracy intervals of method 2. However, this method is also to be used when the number of observations is small.

SCREMOTOX computes the 'observed' load as the mean value determined with one of the three methods, augmented with half the 95% confidence interval. This is in line with the worst case approach.

Table 3.1 The 95% confidence intervals determined for the rivers Rhine and Meuse by De Vries and Klavers (1994)

<table>
<thead>
<tr>
<th>n</th>
<th>river Rhine, Lobith / Cologne</th>
<th>river Meuse, Eijsden</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>chloride</td>
<td>ammonium</td>
</tr>
<tr>
<td></td>
<td>[2a]</td>
<td>[3]</td>
</tr>
<tr>
<td>6</td>
<td>16</td>
<td>26</td>
</tr>
<tr>
<td>12</td>
<td>9</td>
<td>10</td>
</tr>
<tr>
<td>24</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>52</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>100</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>200</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

1) n is the sampling frequency (number/year)

3.2 Transport and retention in surface water

3.2.1 General approach

The surface water system is divided in drainage systems, the river system, the estuary and a number of mixing zones of the North Sea. These compartments shape up a river basin, as is shown in Figure 3.4. The modelling approach to calculate concentrations, retention and transport is different for North Sea zones and the remainder of the river basin. The calculations for the North Sea involve the steady-state version of DELWAQ, a general modelling framework for water and sediment quality applied on the basis of the GENO-grid. The North Sea zones have been selected according to the MANS approach (Waterloopkundig Laboratorium, 1994a).
A simple steady-state box model is used for the land bound parts of river basins. Figure 3.5 gives an overview of the processes considered in both the box model and DELWAQ. Notice the following:

- Dispersion between fresh water compartments and diffusion between water and sediment have been ignored. Diffusion is slow and associated with a small mass flux, when the dissolved concentrations on either side of the water-sediment interface are slightly different in a steady state. Dispersion is fully taken into account for the North Sea.
- Zones in the North Sea are to be defined as subsets of grid cells in such a way, that mass transport across interfaces is minimal in order to get accurate estimates of the contributions of individual loads to the concentrations within a zone.
- Only net settling is considered, which implies that the resuspendable fraction of the sediment is in fact the same material as the fraction that adsorbs micropollutants. The resuspendable fraction has the same particulate concentration of a micropollutant as the suspended matter. This is approximately true in a steady state condition.
- No specification has been given regarding the nature of the decomposition, either photolysis, hydrolysis, oxidation or biodegradation.

The formulations are basically the same for all compartments, the coefficients (input) may be different.

```
zone ..  
| North Sea |
zone -1  v  
| North Sea |
zone 1  v  
| North Sea |
zone 2  v  
| North Sea |
zone ..  v  
| North Sea |
```

Figure 3.1 The compartments and the transportation route in a river basin
3.2.2 Drainage areas, rivers and estuaries

The simplified box approach described below, is appropriate for drainage systems and river systems as long as a system is more or less homogeneous with respect to retention and flushing. This is usually the case in a river system when considered on a seasonal scale. Drainage systems in the same river basin, however, may behave rather differently depending on their specific geographic and hydrological features. Other reasons to distinguish several drainage systems concern differences with respect to:

- the production, application and emission of substances in connection with different laws, directives, standards or practices; and
- the atmospheric transportation route in connection with the geographic position.

Differences may be considerable when drainage systems in a river basin are located in several countries. Nevertheless, the number of drainage systems per river basin in the screening programme is kept to a minimum because of practical reasons. Table 3.2 provides an overview of the river basins selected for SCREMOTOX, and their discharges.

Estuaries may have complicated stratified hydrodynamics, a fresh or brackish toplayer moving out to the sea and a salt water wedge moving upstream. The stratification strongly affects the trapping of suspended matter into the sediment and the related cycling of pollutants between river and sea. These phenomena are ignored within the framework of screening in the sense that stratification and counter flow are not described. However, the compartment specific input must reflect the connected effects, in particular in the loss and flushing rates.
Table 3.2  The river basins discharging into the North Sea and their average flow rates

<table>
<thead>
<tr>
<th>Name river basin</th>
<th>Average flow rate (m³/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Seine</td>
<td>460</td>
</tr>
<tr>
<td>2 Scheldt</td>
<td>110</td>
</tr>
<tr>
<td>3 Rhine (New Waterway)</td>
<td>1650</td>
</tr>
<tr>
<td>4 Meuse (Haringvliet)</td>
<td>930</td>
</tr>
<tr>
<td>5 IJssel (Kornw.+Den Oever)</td>
<td>450</td>
</tr>
<tr>
<td>6 Ems</td>
<td>120</td>
</tr>
<tr>
<td>7 Weser</td>
<td>500</td>
</tr>
<tr>
<td>8 Elbe</td>
<td>1150</td>
</tr>
<tr>
<td>9 Thames</td>
<td>150</td>
</tr>
<tr>
<td>10 Humber</td>
<td>290</td>
</tr>
</tbody>
</table>

The formulations for the box model are separately dealt with for the water column and the upper sediment layer.

**The water column**

The mass balance equation for the water column of a compartment in a steady state is described with:

\[
\text{load - outflow - settling - volatilization - decomposition} = 0
\]

\[
L - Q_0.C_w - F_s.P.f_{dt}.C_w - r_v.f_{st}.C_w.V_w - r_w.C_w.V_w = 0
\]  \hspace{1cm} (3.13a)

\[
F_s = v_s.S_s.(1-f_{st}).A_w
\]  \hspace{1cm} (3.13b)

in which:

- \( A_w \) = surface area of the compartment (m²)
- \( C_w \) = total concentration in the water column (g.m³)
- \( f_{dt} \) = freely dissolved fraction (-)
- \( f_{st} \) = fraction organic carbon in suspended solids excluding phytoplankton (-)
- \( F_s \) = settling flux of suspended organic carbon (g OC.day⁻¹)
- \( L \) = load (g.day⁻¹)
- \( P \) = partition coefficient (10⁶ 1.kg⁻¹ OC)
- \( Q_0 \) = total outgoing flow rate (m³.day⁻¹)
- \( r_v \) = volatilization rate (day⁻¹)
- \( r_w \) = first order decomposition rate in the water column (day⁻¹)
- \( S_s \) = concentration of suspended solids excluding phytoplankton (g.m³)
- \( v_s \) = net settling velocity (m.day⁻¹)
- \( V_w \) = water volume (m³)
Some parameters in equation 3.13 are aggregate parameters, which are quantified from other simple algebraic relations. Load L is composed of discharges of pollution sources, the discharge from the upstream compartment and the atmospheric deposition. The outgoing flow rate Q₀ may be the sum of several flow rates going to as many downstream compartments (grid cells or zones in the North Sea).

The settling flux Fₛ is actually the sum of contributions of suspended matter and phytoplankton. However, the contribution of phytoplankton settling is neglected, which is justifiable because of very small settling velocities. The detritus settling resulting from phytoplankton mortality is taken into account as part of the suspended matter settling, expressed in organic carbon units (OC).

The dissolved fraction fₓ is derived from the partitioning of a substance between water, dissolved organic matter, (organic) suspended matter and phytoplankton. Not only dissolved fractions, but also particulate fractions are deduced using partition coefficients (see section 3.4).

The volatilization rate rᵥ is a function of substance and compartment specific coefficients:

\[
rv = (h(1/k_l + 1/(H_{a1}.k_g)))^{-1} \tag{3.14}
\]

\[
H_{a1} = H_{a2}.(R.(T_a + 273.15))^{-1} \tag{3.15}
\]

in which:

\begin{align*}
h & = \text{depth of water column (m)} \\
H_{a1} & = \text{dimensionless Henry’s constant at average temp. (mol.m}^3\text{)(mol.m}^3\text{)}^{-1} \\
H_{a2} & = \text{Henry’s constant at average ambient temperature (Pa.m}^3\text{.mol}^{-1} \\
k_g & = \text{mass transfer coefficient in the gas film (m.d}^{-1}\text{), compartment specific} \\
k_l & = \text{mass transfer coefficient in the liquid film (m.d}^{-1}\text{), compartment specific} \\
R & = \text{gas constant (8.3 Pa.m}^3\text{.mol}^{-1}\text{.K}^{-1}) \\
T_a & = \text{average ambient temperature (10 °C)}
\end{align*}

The decomposition rate rₓ is substance and compartment specific. The parameters rₓ and Hₑ₂ are temperature dependent, approximately according to:

\[
\text{par}_r = \text{par}_{r20}.T_c^{(T_a-20)} \tag{3.16}
\]

in which:

\begin{align*}
\text{par}_{r20} & = \text{H or } rₓ \text{ at a temperature of 20 °C} \\
T_c & = \text{temperature coefficient (approximately 1.07)}
\end{align*}
Equation 3.13 is converted to yield the total concentration in the water column:

\[ C_w = \frac{L}{(V_w \cdot (rf + rl + r_w))} \]  \hspace{1cm} (3.17)

in which:
- \( rf \) = flushing rate or reciprocal hydraulic residence time (Qo/Vw; day⁻¹)
- \( rl \) = total physical loss rate (Fs.P.fgr/Vw + r_r.fgr; day⁻¹)

The fraction of the load of a substance retained in a compartment in steady state is equal to the ratio of the total mass flux of the loss processes and the load:

\[ fret = \frac{(rl + r_w)}{(rf + rl + r_w)} \]  \hspace{1cm} (3.18)

The fractions of the load distributed into several downstream compartments are given by:

\[ fdis_i = flush_i \cdot (1 - fret) \]  \hspace{1cm} (3.19)

in which:
- \( flush_i \) = partial flushing ratio (Qo/Qo)

The fraction volatizing into the atmosphere, the fraction settling into the sediment and the decomposed fraction are respectively described by:

\[ fatm = \frac{rv.fgr.fret}{(rl + r_w)} \]  \hspace{1cm} (3.20)
\[ fset = \frac{Fs.P.fgr.fret}{(V_w \cdot (rl + r_w))} \]  \hspace{1cm} (3.21)
\[ fdec = fret - fatm - fset \]  \hspace{1cm} (3.22)

All these factors are expressed as percentages in the output of the screening programme. They are used to determine the corresponding mass fluxes from the load.

The determination of the percentual contributions of the individual sources of pollution in the total load on or the concentration in a compartment is straight forward for the land bound compartments. This is just a matter of bookkeeping, starting at the most upstream compartment. Tracking down the sources of pollution in zones of the North Sea is more complicated with respect to the aquatic route as feedback occurs through large scale circulations and dispersive transport depends on gradients reflecting overall loading. This problem has been approximately solved by making separate DELWAQ-simulations for the discharge of each river basin. A relative contribution is then estimated as the ratio of the 'partial' concentration and the sum of all 'partial' concentrations.
The sediment layer

The mass balance equation for the upper sediment layer of a compartment in a steady state is described with:

\[ \text{settling - burial - decomposition} = 0 \]

\[ \text{fset}_L - r_b \cdot C_s - r_s \cdot C_s \cdot V_s = 0 \]  \hspace{1cm} (3.23)

\[ r_b = \frac{\text{Fs}(1 - a_0 \cdot f_{sc})}{f_{sc} / ((1-f_{sand})(1-\phi))} / D \]  \hspace{1cm} (3.24)

in which:
\[ a_0 = \text{conversion factor from organic carbon to organic matter} (=1.7) \]
\[ C_s = \text{total concentration in bulk sediment} \ (\text{g.m}^3) \]
\[ D = \text{density of sediment} \ (\text{approx: } 2.5 \times 10^6 \ \text{g.m}^3) \]
\[ f_{sc} = \text{fraction organic carbon in the settled material} (-) \]
\[ f_{sand} = \text{fraction of sand in settled material} (-) \]
\[ r_b = \text{burial rate} \ (\text{m}^3.\text{day}^{-1}) \]
\[ r_s = \text{first order decomposition rate in the sediment} \ (\text{day}^{-1}) \]
\[ V_s = \text{bulk sediment volume} \ (\text{m}^3) \]

The load fset. L is determined as an average value on a yearly basis, as the time-scale of the sediment processes is in the order of decades. This implies the averaging of seasonal loads. Moreover, the fraction of sand in the settled material represents the non-adsorbing fraction. Both fractions \( f_{sc} \) and \( f_{sand} \) are compartment specific, whereas decomposition rate \( r_s \) is also substance specific and temperature dependent.

Notice the assumption that all settled organic matter is decomposed in the upper sediment layer, which is only approximately true. The burial flux is equal to zero, when settled material is only composed of organic matter. The influx of micropollutant into the sediment is then in fact the result of the biogenic incorporation of organic matter temporarily settled at the sediment.

Equation 3.23 is converted to yield the total concentration in the sediment layer:

\[ C_s = \frac{\text{fset}_L}{V_s \cdot r_s + r_b} \]  \hspace{1cm} (3.25)

It is obvious that the fraction of sand in the settled material must always be smaller than 1 (conform the real world). Moreover, this equation cannot be solved when only organic matter settles and the micropollutant is not subjected to decomposition. The screening programme estimates the particulate concentration in such a case on the basis of partitioning using the dissolved concentration in the water column as a reference.
The partitioning among particles, pore water and biota is determined in a similar way as in case of the water column.

The fraction buried into the sediment and the decomposed fraction are respectively described by:

\[
\begin{align*}
\text{fbur} &= \frac{r_b C_s}{(\text{fset.L})} \\
\text{fdec} &= \frac{V_r r_r C_s}{(\text{fset.L})}
\end{align*}
\]

Both factors are expressed as percentages in the output of the screening programme. They may be used to determine the corresponding mass fluxes from the load.

### 3.2.3 The North Sea

The main problems that occur when applying simplified steady-state approaches to (mixed zones of) the North Sea relate to long time-scales, feed-back and dispersion. The causes can be described as follows:

- Hydraulic residence times in zones of the North Sea are usually longer than 3 months (a season), so that a seasonal steady state does not actually occur. Even worse, a seasonal steady state in an upstream zone is not linked up with the steady state for the same season in a downstream zone because of delay.
- Feed-back arises when large circulations will eventually cause the inflow of substances from an upstream zone originating from a river load discharged into a downstream zone.
- Dispersive transport connected with gradients establishes the loss or inflow of mass into or from the outer boundaries of compartments.

Ignoring these problems inevitably leads to poorly defined inaccuracy in the calculated concentrations. It was therefore decided to incorporate steady-state DELWAQ into the screening instrument. This eliminates two of the three above causes of inaccuracy. The first mentioned cause remains. However, one must keep in mind the purpose of the methodology, which is the screening of substances referring to the highest computed concentrations. Exact time-dependent computations are therefore not needed. It can be argued that worst case calculations are possible without serious overestimation of concentrations in target zones. Important features of the simulation with DELWAQ are:

- The water quality simulation is based on the 2x2 aggregated GENO schematization. The spatial resolution is 16x16 km, which results in approximately 1400 computational elements for the North Sea area considered.
- The southern boundary of the North Sea system has been positioned between Cherbourg and Southampton, the northern boundary between Aberdeen and Hanstholm (Denmark).
- A long-term residual hydrodynamic flow field is used as basis for transport. The hydrodynamic calculation is performed by the model WAQUA based on a long-term averaged windcondition (South west, 7.4 m/s).
• 10 river basins have been distinguished for the WAQUA-simulation, each having yearly averaged flow rates. The contribution of the river discharges to the North Sea transport fluxes is small. Seasonal variation in the riverflows will therefore have limited influence on the calculated concentrations in the computational elements. Seasonal variation in the discharges of a substance concentrations is accounted for in the loads.

• The formulations of water quality processes are in agreement with those of the simplified box model.

• Forcing functions like suspended solids and DOC and parameters like the settling velocity have been specified for each zone.

The results of the model for the computational elements cells are aggregated into 15 zones. These zones have been selected conform the MANS study (Waterloopkundig Laboratorium, 1994a) on the basis of three criteria. Zones are rather well mixed, are more or less homogeneous with respect to settling, water mass and water depth, and have a specific value as ecosystem and/or resource area. The zones are specified in Table 3.3 and in Figure 3.6.
A complication in the DELWAQ-application arose from the demand to determine the contribution of the sources of emission to the mass of a substance in a North Sea zone. This was solved in a pragmatic but successful way as was shown in previous studies. Separate simulations are made for each of the river basin discharges, for the aggregate atmospheric sources and for each of the in-situ sources. The masses in a zone resulting from the individual sources are added to deliver the total mass, that would approximately result from a simulation for simultaneous loading from all sources. The ratios of the masses resulting from individual sources and the total mass have appeared to be good approximations of the contributions of the sources.

The contribution of an aggregate source is split up further into the partial contributions of individual sources. This proceeds through accounting of the loads on river basin compartments calculated with the box model and of the atmospheric loads from countries calculated with the emission module.

Table 3.3  The North Sea zones, their surfaces areas and volumes

<table>
<thead>
<tr>
<th>Number</th>
<th>Name</th>
<th>Surface (km²)</th>
<th>Volume (km³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>North English coast</td>
<td>23600</td>
<td>905</td>
</tr>
<tr>
<td>2</td>
<td>English Channel</td>
<td>33300</td>
<td>1089</td>
</tr>
<tr>
<td>3</td>
<td>Central North Sea</td>
<td>137000</td>
<td>8450</td>
</tr>
<tr>
<td>4</td>
<td>South English coast</td>
<td>9220</td>
<td>157</td>
</tr>
<tr>
<td>5</td>
<td>Southern North Sea</td>
<td>24600</td>
<td>769</td>
</tr>
<tr>
<td>6</td>
<td>Dogger bank</td>
<td>10500</td>
<td>296</td>
</tr>
<tr>
<td>7</td>
<td>Flemish banks</td>
<td>3840</td>
<td>65</td>
</tr>
<tr>
<td>8</td>
<td>Zeeland coast</td>
<td>4100</td>
<td>71</td>
</tr>
<tr>
<td>9</td>
<td>Oystergrounds</td>
<td>30200</td>
<td>1292</td>
</tr>
<tr>
<td>10</td>
<td>Frisian front</td>
<td>9220</td>
<td>336</td>
</tr>
<tr>
<td>11</td>
<td>Dutch coast</td>
<td>5380</td>
<td>94</td>
</tr>
<tr>
<td>12</td>
<td>Wadden coast</td>
<td>7170</td>
<td>149</td>
</tr>
<tr>
<td>13</td>
<td>East North Sea</td>
<td>16400</td>
<td>614</td>
</tr>
<tr>
<td>14</td>
<td>German Bight</td>
<td>22300</td>
<td>817</td>
</tr>
<tr>
<td>15</td>
<td>Ger/Dan coast</td>
<td>20700</td>
<td>331</td>
</tr>
</tbody>
</table>

3.3  Transport and retention in the atmosphere

Atmospheric deposition can be an important source of contamination for the North Sea. However, detailed information on atmospheric transport and deposition of individual substances is not available, except for a few heavy metals and organic micropollutants, for which deposition was estimated in modelling studies performed by TNO-MW. Estimating deposition must therefore be based on results from these studies, connecting emissions on land with atmospheric deposition on the North Sea.

However, important structural differences exist between heavy metals and organic substances. Heavy metals are often emitted continuously, the emission of organic micropollutants such as pesticides may have a seasonal time scale. Moreover, in contrast with heavy metals, organic substances may be decomposed as the consequence of (photo)chemical reactions.
The geographical position of emissions is important for the extent of deposition on the North Sea or on any other specific area. However, exact positions will not (easily) be available in many cases. A practical solution to this problem is to aggregate the emissions from drainage systems on a national or supranational level.

Over 90% of dry and wet deposition on the North Sea results from emissions in North-West Europe for most compounds. However, global background concentrations might contribute significantly to deposition for compounds with atmospheric residence times larger than approximately three weeks. Given the physico-chemical properties of a substance, it can be assessed whether this substance has a potential for spreading across the globe through the atmosphere.

Considering the above, the following starting points were determined for the formulation of the atmospheric deposition in SCREMOTOX:

- Depending on available data, the atmospheric emissions \( E_{mi} \) (ton.y\(^{-1}\)) may be aggregated for:
  - the European Community and the aggregate rest of Europe;
  - a selection of EC-countries (for example North-West Europe, including Germany, the Netherlands, Belgium, Luxembourg, France and the United Kingdom), the other individual EC-countries and the aggregate rest of Europe; or
  - individual countries, that is the Netherlands, Germany, France, Belgium, Luxembourg, United Kingdom, Denmark, Norway, Sweden, Ireland and Spain, and the aggregate emission of the rest of Europe.

- The atmospheric deposition on the North Sea is calculated relative to heavy metal fluxes determined in the previous TNO-study, if necessary, corrected for (photo-)chemical degradation of the gaseous fraction.

- The deposition is based on yearly or seasonally average emissions and yearly meteorology.

- The deposition flux is specified according to zones, taking into account the travel times between countries and zones with regard to degradation.

- A 'background' deposition related to emissions in remote parts of the world may be imposed on the North Sea, next to the 'direct' deposition resulting from emissions in Europe.

The estimation of atmospheric emissions is described in section 3.1.

### 3.3.1 Atmospheric deposition of emissions in Europe

The atmospheric deposition on a North Sea zone is calculated with:

\[
L_{ai} = \sum_{x=1}^{n} (E_{mi} \cdot D_{ix} \cdot (\phi + (1-\phi) \cdot e^{-\alpha_{ix} t_{ix}})) \cdot A_i / A
\]

(3.28)
in which:

- \( A \) = surface area of the North Sea (m\(^2\))
- \( D_f \) = fraction of deposition on the North Sea (-)
- \( E_m \) = total emission quantity (g.day\(^{-1}\))
- \( L_a \) = atmospheric load (g.day\(^{-1}\))
- \( r_a \) = degradation rate (day\(^{-1}\))
- \( t \) = average travel time (day)
- \( \phi \) = ratio aerosol-adsorbed concentration and total atmospheric concentration (-)

Index \( x \) relates to individual countries or groups of countries
Index \( z \) relates to zones

The deposition fractions \( D_f \) of organic substances used for SCREMOTOX are based on results of a previous study (Baart et al., 1995), that is the overall deposition fractions on the North Sea of heavy metals emitted from individual countries (see Table 3.4). In this study atmospheric deposition on the North Sea was calculated based on yearly averaged European emissions. The model used in that study is EUTREND (version 1.13), which covers the entire European continent with its marginal seas. It has a variable spatial resolution; it was applied using a fixed receptor grid over the North Sea with a 0.5\(^\circ\) long. x 0.25\(^\circ\) lat. resolution. This Langrangian type model is driven by meteorological data obtained through the Netherlands Meteorological Institute (KNMI) and from the European Centre for Medium Range Weather Forecasts (ECMWF) in England, in combination with synoptic surface observations from more than 1500 stations in Europe.

An important aspect with regard to dispersion and advection is that EUTREND describes long range air transport using well mixed trajectories, whereas local transport and dispersion is described using a Gaussian plume description. Atmospheric processes in the model included advection, dispersion, chemical degradation, and dry and wet deposition. Dry deposition refers to both the deposition of aerosols and the gas-water exchange. Wet deposition relates to the precipitation of rainwater, scavenging both gaseous and aerosol-bound compounds from the atmosphere.

Applying the heavy metal deposition fractions to organic compounds with similar aerosol-dominated deposition will lead to marginal errors. For compounds which tend to be in the gaseous phase deposition fluxes may be different. Relatively little is known about dry deposition velocities for most persistent organic compounds. Partial dry deposition (gas-water exchange) velocities over sea can be estimated according to Liss and Slater (1974). The velocities of relatively volatile organic compounds are thought to vary between 1.0 and 0.01 cm/s, based on atmospheric resistance. However, results for organic compounds remain uncertain (by at least a factor 5) as experimental verification remains very difficult.

Correction of the deposition for differences connected with the transport over land seem infeasible. Type of vegetation, soil, humidity and concentration of the compound in the soil all influence surface-air exchange. There are, yet, no experimentally tested estimation models for dry deposition velocities on soil/vegetation for organic compounds.

Considering the above, it was decided not to implement corrections of the total deposition flux regarding the various forms of deposition in the first version of SCREMOTOX.
Table 3.4 The deposition fractions of heavy metals for the North Sea (Baart et al., 1995)

<table>
<thead>
<tr>
<th>Deposition fraction</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Europe</td>
<td>2.0</td>
</tr>
<tr>
<td>North-West Europe</td>
<td>7.0</td>
</tr>
<tr>
<td>The Netherlands</td>
<td>9.2</td>
</tr>
<tr>
<td>Belgium and Luxembourg</td>
<td>4.3</td>
</tr>
<tr>
<td>Germany</td>
<td>2.4</td>
</tr>
<tr>
<td>United Kingdom</td>
<td>16.0</td>
</tr>
<tr>
<td>France</td>
<td>2.3</td>
</tr>
<tr>
<td>Denmark</td>
<td>6.5</td>
</tr>
<tr>
<td>Norway</td>
<td>5.4</td>
</tr>
<tr>
<td>Sweden</td>
<td>1.3</td>
</tr>
<tr>
<td>Ireland</td>
<td>6.0</td>
</tr>
<tr>
<td>Spain</td>
<td>0.2</td>
</tr>
<tr>
<td>Other countries</td>
<td>0.1</td>
</tr>
</tbody>
</table>

The degradation of aerosol-bound compounds is considered unimportant. This is obviously the case for heavy metals. However, deposition of compounds prone to chemical degradation will be overestimated if the Df,-factors for heavy metals are used without correction. The distribution of a substance among aerosols and the gaseous phase is mainly determined by vapour pressure and temperature. The distribution can be estimated with the following equation according to Junge (1977):

$$\Phi = c\Theta(p^0L + c\Theta)^{-1}$$  \hspace{1cm} (3.29)

in which:

- $\Theta$ = the aerosol surface area $1.5 \times 10^4 \text{m}^2 \cdot \text{m}^3 \text{air}$ (average background concentration)
- $p^0L$ = the solute saturation vapour pressure (Pa)
- $c$ = a constant depending on heat of condensation and molecular weight (Junge assumed 0.17 Pa for high molecular weight organics)

The most important loss reaction of most gaseous organic compounds in the atmosphere is the second-order reaction with the OH-radical. The degradation rate is equal to:

$$r_s = 86400 \, k_{OH} \cdot [\text{OH}]$$  \hspace{1cm} (3.30)

with:

- $k_{OH}$ = reaction constant ($\text{cm}^3\cdot\text{molec}^{-1}\cdot\text{s}^{-1}$)
- $[\text{OH}]$ = average atmospheric OH-radical concentration; $5 \times 10^5 \, \text{molec. cm}^{-3}$

For most organic compounds chemical degradation rates can be estimated (Atkinson, 1986).

The travel time can be calculated from an averaged source-receptor distance and an average windspeed ($u = 10 \, \text{m/s}$). The distance is adapted for non-linearity of air-mass trajectories with an average factor 1.5.
3.3.2 Background deposition on the North Sea

SCREMOOTOX assesses the need to impose a background deposition on the basis of the atmospheric residence time of a substance, which depends on two major loss processes, namely (photo)chemical degradation of gaseous compounds in the atmosphere and deposition. Both are strongly dependent on the tendency of substances to adsorb onto aerosols. Aerosol-bound compounds are less sensitive to photochemical degradation than gaseous compounds. Moreover, such compounds are not prone to long distance transportation, because aerosols are relatively rapidly deposited. Long distance transport is not important when the deposition velocity is higher than 0.1 cm/s.

Criteria have therefore been derived from the gas-aerosol distribution $\phi$ (see equation 3.29) and the half life time regarding degradation $T_{0.5}$. It is recommended to impose a background deposition when $\phi > 0.10$ and $T_{0.5} > 20$ days. The background deposition may be ignored when these conditions are not fulfilled.

The half life time $T_{0.5}$ is derived from the second order degradation rate with:

$$T_{0.5} = \frac{86400 \ln 2}{(k_{OH} [OH])} \quad (3.31)$$

Background deposition can be imposed in SCREMOOTOX by providing:

1) the deposition flux to the North Sea due to global background concentrations; or
2) a background concentration over the North Sea.

In case 2, SCREMOOTOX calculates the deposition flux by multiplication of the background concentration with an average overall deposition velocity of 0.3 cm.s$^{-1}$ (TNO, 1995b).

3.4 Partitioning and exposure

Mean equilibrium concentrations

Partitioning among the dissolved and particulate phases affects the loss and distribution of a substance as well as the exposure of organisms to this substance. Partitioning is formulated according to the equilibrium concept of partition coefficients. The total concentration of an organic micropollutant is the sum of four contributions:

$$C_t = (f_{poc} + f_{phyt} + f_{doc} + f_{ad}) \cdot C_t \quad (3.32)$$

in which:

- $C_t$ = total concentration (g.m$^{-3}$), $C_w$ or $C_s$
- $f_{ad}$ = freely dissolved fraction (-)
- $f_{doc}$ = fraction adsorbed to dissolved organic matter (-)
- $f_{phyt}$ = fraction adsorbed to phytoplankton (-)
- $f_{poc}$ = fraction adsorbed to the organic part of (suspended) matter (-)
All organic matter is expressed in amounts of carbon. The fractions are derived from a partition coefficient defined according to:

\[ P = \frac{C_p}{(f_{df} \cdot C_p)} \]  

(3.33)

in which:

\( C_p \) = particulate concentration (g.g\(^{-1}\) OC)
\( P \) = partition coefficient (m\(^3\).g\(^{-1}\) OC = 10\(^{-4}\) l.kg\(^{-1}\) OC)

The partition coefficient (P) is usually available as \( K_{oc} \) (l.kg\(^{-1}\)), the conversion of which into P requires a multiplier of 10\(^{-4}\). Linear relations are available to estimate \( K_{oc} \) on the basis of the octanol–water partition coefficient (\( K_{ow} \); l.kg\(^{-1}\)).

The fractions follow from:

\[ f_{df} = \phi / (\phi + P \cdot C_{toc}) \]  

(3.34)

\[ f_{poc} = (1-f_{df}) \cdot C_{poc}/C_{toc} \]  

(3.35)

\[ f_{phyt} = (1-f_{df}) \cdot C_{phyt}/C_{toc} \]  

(3.36)

\[ f_{doc} = (1-f_{df}) \cdot X_{doc} \cdot C_{doc}/C_{toc} \]  

(3.37)

\[ C_{poc} = f_{oc} \cdot S_s \]  

(3.38)

\[ C_{toc} = C_{poc} + C_{phyt} + X_{doc} \cdot C_{doc} \]  

(3.39)

in which:

\( C_{doc} \) = dissolved organic carbon concentration (g OC.m\(^{-3}\))
\( C_{phyt} \) = phytoplankton concentration (g OC.m\(^{-3}\))
\( C_{toc} \) = total organic carbon concentration (g OC.m\(^{-3}\))
\( f_{oc} \) = fraction organic carbon in suspended solids excluding phytoplankton (-)
\( S_s \) = (suspended) sediment concentration excluding phytoplankton (g.m\(^{-3}\))
\( X_{doc} \) = sorption efficiency relative to particulate organic carbon (-)
\( \phi \) = porosity (-), which is equal to 1 in the water column

Combining the fractions with the total concentration yields the individual probable exposure concentrations (PEC) in water, particulate matter and phytoplankton. It is obvious that the phytoplankton contribution is not relevant for the sediment layer.

Similar formulations can be used for heavy metals, but then sorption is considered relative to the total mass of (suspended) sediment in stead of its organic part. Different partition coefficients may be used for sorption to sediment and phytoplankton.
Assuming that the amount of mass of a substance taken up in other biota than phytoplankton is small compared to the total concentration, the exposure concentration in biota is derived directly from the dissolved concentration with:

\[ C_b = f_{fp} \cdot BCF \cdot C_d \]  \hspace{1cm} (3.40)

in which:
- BCF = bioconcentration factor (m³.g lipids)
- \( C_b \) = concentration in biota (g.g⁻¹ fresh weight)
- \( C_d \) = total dissolved concentration (g.m⁻³)
- \( f_{fp} \) = fraction lipids in fresh weight (-)

Data for the lipid fraction of relevant marine species groups are presented in Table 3.5. Few data are available on bioconcentration factors. However, a BCF can be estimated from in a similar way as the partition coefficient with \( BCF = 10^6 \cdot K_{ow} \). This is based on the following assumptions:

- partition between animal fat tissue and water is regulated by diffusion processes;
- the animal fat tissue can be regarded as a physio-chemical homogeneous phase;
- the average molar volumes of fat molecules in animals and the 'lipid model' octanol are comparable.

Table 3.5 Typical lipid fractions for marine organism

<table>
<thead>
<tr>
<th>Species group</th>
<th>Lipid fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Algae</td>
<td>12.5%</td>
</tr>
<tr>
<td>Bivalves</td>
<td>11.5%</td>
</tr>
<tr>
<td>Amphipods</td>
<td>19.0%</td>
</tr>
<tr>
<td>Echinoderms</td>
<td>24.3%</td>
</tr>
<tr>
<td>Roundfish</td>
<td>49.5%</td>
</tr>
<tr>
<td>Eel</td>
<td>51.6%</td>
</tr>
</tbody>
</table>

References: Jørgensen et al., 1991; Geyer et al., 1993; Hill et al., 1992; Xu et al., 1989; Gobas et al., 1993; Geyer et al., 1994; Fox et al., 1994

**Variability**

The dynamic input and dispersion of a substance into the marine environment establishes a concentration distribution, or in other words, variability in the concentration. The reference for a risk assessment should rather be this concentration distribution than an average concentration. The exposure used in risk analysis is therefore linked up with the mean value and the 95-percentile upper boundary value of a normal concentration probability function. Such functions are derived for each North Sea zone from the concentrations computed with the North Sea Shelf model (DELWAQ) for each grid cell in a zone.
Uncertainty

The uncertainty is quantified as a possible increase of the concentrations, due to the uncertainty in the physico-chemical substance characteristics that determine the rates or equilibria of processes. The maximal values of the exposure concentrations follow from a worst case computation with SCREMOTOX, using an appropriate setting of high and low estimates for the substance characteristics. The relevant parameters are partition coefficients, Henry’s constant and decomposition rates.

Input to the risk assessment

The risk assessment is based on the 95-percentile exposure concentrations for both the most probable combination of substance characteristics and the worst case combination.

3.5 Ecotoxicological risk

3.5.1 Risk assessment

The ecotoxicological risk caused by the exposure of an organism to a toxic substance is defined as the ratio of a probable exposure concentration (PEC) and a specific effect concentration (EC), also indicated here as test value. The selected test values are:

- EC₅₀: acute toxic effects concentration, resulting in an effect for 50% of the individuals in a test population or in a 50% reduction of an effect parameter;
- NEC: no effects concentration, related to the Dutch Maximal Permissible Risk Concentration (MPRC);
- 0,01 NEC: no effects concentration, including an additional safety factor for overall uncertainty (e.g. extrapolation from lab to field) and possible combination toxicity, related to the Dutch Negligible Risk Concentration (NRC).

Each of the test values applies to three exposure-effect routes:

- uptake from the water by pelagic organisms (NEC_water);
- uptake from (suspended) sediment by benthic organisms (NEC_sediment); and
- uptake by higher organisms through the food chain (NEC_bio).

Ranking substances for ecotoxicological risk according to a PEC/effect concentration has the disadvantage that the uncertainties in PEC and effect-concentrations may have a large bearing on the results. A less sensitive method of ranking was found in classification. Using three test values allows the definition of the following four classes:

1. PEC < 0,01 NEC
2. NEC > PEC > 0,01 NEC
3. EC₅₀ > PEC > NEC
4. PEC > EC₅₀
The ranking of substances can now be done according to class numbers. Risk assessment takes the following steps:

- determination of the three ratios of PEC and effect concentrations;
- ranking of the North Sea zones and seasons according to the PEC/NEC ratio; and
- attribution of a class number to the case/substance on basis of the highest computed value of the PEC for all zones and seasons.

### 3.5.2 Determination of effect concentrations

The test values (NEC, etc.) for each of the exposure-effect routes can be given independent values in the input for SCREMOTOX. However, it is to be expected that data will not be available for all three values in many cases. If only one of the values is available, the other two can be deduced from this value using the equilibrium partitioning relations (see section 3.4).

Lowest available values are to be selected for the $EC_{50}$. Procedures to determine the NEC for three exposure-effect routes are described in the next sections. The procedures have not yet been incorporated in the computer program of SCREMOTOX.

#### General

The NEC is a measure for the sensitivity of the ecosystem. It represents the concentration of a chemical in the environment below which no direct adverse effects will occur. The NEC is determined by extrapolation from experimental ecotoxicological data. During recent years a number of methods for determination of the NEC have been developed (TNO, 1995e). The OECD method is adopted within this project because of its international acceptance. In this method, the lowest available (and acceptable) figure is selected and an empirical safety factor is applied to this figure. The magnitude of this safety factor is dependent upon the type of data (chronic NOEC or acute $EC_{50}$) and the representativeness of data for algae, crustaceans and fish.

#### NEC for evaluation of exposure through the water phase

The OECD method for determining a NEC for aquatic biota requires NOECs from chronic toxicity tests or $EC_{50}$s from acute toxicity tests. In the screening method developed here this requirement is not used *sensu stricto* because there is no internationally accepted definition of chronic or acute exposure. It is proposed to evaluate whether or not a test might be considered to be acute on the basis of expert opinion. This will proof to be no problem because the number of chronic toxicity tests with ‘not well known’ chemicals is extremely low.
The present OECD scheme (OECD, 1993a) has not been designed for use in all situations. If one or two chronic NOECs are available and less than three representative EC_{50}s, it is not clear how a NEC must be calculated with this scheme. On the basis of a discussion with OECD-representatives in the Netherlands, Norway and the United Kingdom (within the framework of the CHARM project) the scheme which is presented in Table 3.6 was composed to allow calculation of a NEC for all scenarios in which aquatic toxicity data are available. It is thought to be impossible to produce a reliable estimate of the NEC when ecotoxicological data are not available at all. The scheme of Table 3.6 resembles the logical structure of the OECD method.

Table 3.6: The OECD scheme for the calculation of a NEC for aquatic exposure. On the x-axis the availability of 'acute' EC_{50}'s is listed and on the y-axis the availability of 'chronic' NOECs. In case of an 'or' statement, the lowest value is used.

<table>
<thead>
<tr>
<th>NOECs</th>
<th>EC_{50}'s</th>
</tr>
</thead>
<tbody>
<tr>
<td>data for at least algae,</td>
<td>data, but not for algae,</td>
</tr>
<tr>
<td>crustaceans and fish</td>
<td>crustaceans and fish</td>
</tr>
<tr>
<td>NOEC/10</td>
<td>no data</td>
</tr>
<tr>
<td>NOEC/10 or EC_{50}/100</td>
<td>calcul. not meaningful</td>
</tr>
<tr>
<td>no data</td>
<td>calculation impossible</td>
</tr>
</tbody>
</table>

Data on all generally accepted effect parameters (e.g. mortality, growth, etc.) are used. For each species the value resulting from the logarithmic mean (of the different tests) for the most sensitive effect parameter is used as an input to the scheme.

**NEC for evaluation of exposure through sediment**

At the 1991 OECD workshop on effects assessment of chemicals in sediments (OECD, 1993a), three methods were recommended for the development of sediment quality objectives: equilibrium partitioning, interstitial water quality and spiked sediment testing. It is proposed that within the screening method, the calculation of the NEC_{benthic} is always based on toxicity data for, if possible, spiked sediments. If no toxicity data from sediment tests are available, a sediment NEC must not be calculated.

By using the rules presented in Table 3.6, a NEC_{benthic} is generally calculated from the lowest EC_{50}/1000.

**NEC for evaluation of exposure through food**

A scheme is presented in the ‘Guidance document for aquatic effects assessment’ (OECD, 1993), which can be rearranged in a form comparable to the one for aquatic toxicity (Table 3.8). The method arises from discussions which took place in The Netherlands and has not yet been discussed by the OECD. Again, the assessment factor is applied to the lowest value. If no test data for exposure through food are available no NEC_{benthic} will be calculated.
An LC$_{50}$ for dietary exposure (mg kg$^{-1}$ fresh weight, preferably 5 days) is preferred over LD$_{50}$ (mg) values for single oral dose tests. If not available, LC$_{50}$ values (lethal concentration) can be estimated from LD$_{50}$ values (lethal single oral dose) by multiplying them with a conversion factor given in Table 3.7 (OECD, 1993a).

Table 3.7: Conversion factors for conversion of LD$_{50}$ values into LC$_{50}$ values

<table>
<thead>
<tr>
<th>Species</th>
<th>Conversion factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Canus domesticus</td>
<td>40</td>
</tr>
<tr>
<td>Macaca spec.</td>
<td>20</td>
</tr>
<tr>
<td>Microtus spec.</td>
<td>8.3</td>
</tr>
<tr>
<td>Mus musculus</td>
<td>8.3</td>
</tr>
<tr>
<td>Oryctolagus cuniculus</td>
<td>33.3</td>
</tr>
<tr>
<td>Rattus norvegicus (age &gt; 6 weeks)</td>
<td>20</td>
</tr>
<tr>
<td>Rattus norvegicus (age &lt; 6 weeks)</td>
<td>10</td>
</tr>
</tbody>
</table>

Table 3.8 The scheme for the calculation of a NEC for exposure via the food chain. On the x-axis the availability of acute EC$_{50}$ is listed and on the y-axis the availability of chronic NOECs. In the case of an 'or' statement, the lowest value is used.

<table>
<thead>
<tr>
<th>NOECs</th>
<th>EC$_{50}$'s</th>
</tr>
</thead>
<tbody>
<tr>
<td>data for _ 3 species</td>
<td>data for 1 or 2 species</td>
</tr>
<tr>
<td>data for _ 3 species</td>
<td>NOEC/10</td>
</tr>
<tr>
<td>data for 1 or 2 species</td>
<td>NOEC/10 or EC$_{50}$/100</td>
</tr>
<tr>
<td>no data</td>
<td>EC$_{50}$/100</td>
</tr>
</tbody>
</table>

EC$_{50}$'s calculation not meaningful

Required data

The following data have to be collected for a proper determination of effect concentrations:

- **Species name**
  This is the name of the species that has been tested with the current chemical. You can enter all names (scientific or English), as long as the same species is always given the same name. Frequently used test species are:

  **Water**
  *Skeletonema costatum* (Algae)
  *Scenedesmus subspicatus* (Algae)
  *Seleniastrum capricornutum* (Algae)
  *Acartia tonsa* (Crustaceans)
  *Daphnia magna* (Crustaceans)
  *Mysisopsis bahia* (Crustaceans)
  *Nitocra spinipes* (Crustaceans)
**Oncorhynchus mykiss** (Fish)
**Brachidiono rerio** (Fish)
**Pimephales promelas** (Fish)

**Sediment**
*Abra alba* (Molluscs)
*Arenicola marina* (Annelids)
*Corophium volutator* (Crustaceans)

**Foodchain**
*Rattus norvegicus* (Mammals)
*Cans domesticus* (Mammals)
*Microtus spec.* (Mammals)

- **Taxonomic group**
  The taxonomic group may be 'Algae', 'Crustaceans', 'Molluscs', 'Fish' or 'Other'.

- **Effect type**
  The effect type measured in the toxicity test has to be specified.

- **Exposure time**
  The exposure time is the duration of the toxicity test.

- **Effect size**
  The size of the effect concerns the effect (%) measured in the toxicity test. Only EC_{50}’s and NOEC’s can be used for SCREMOFOX.

- **Concentration**
  This is the concentration that caused the measured effect.

- **Exposure route**
  The test species can be exposed to the chemical through the water, the sediment or it’s food.

- **Fresh/Salt water**
  In case ‘water’ is the exposure route, the type of water used in the test must be specified.

### 3.6 Input

The input consists of user-defined input and prefixed input. The user-defined input relates to options, physico-chemical substance characteristics, effect concentrations and emissions. The prefixed input mainly concerns the parameters determining the transport and retention of substances in the various compartments of the natural system.
Options

The selection of options proceeds through a question-decision procedure, forcing the user to think about:

- how to produce optimal input;
- choosing a path through the computation; and
- the necessity to interrupt and to terminate the computation.

The latter refers to the following in particular. SCREMOTOX makes a prognosis of the risks (PEC/NEC) for individual zones after having quantified the various loads into the North Sea. The program communicates whether the expected risks are significant or not. Further computations may be abandoned if no risk is to be expected. The expected exposure concentration in a North Sea zone i is estimated with:

\[
\text{PEC}_i = \frac{L_i \cdot T_i}{V_i} \quad (3.41)
\]

\[L_i = \sum_{j=1}^{n} F_{r_{ij}} \cdot E_j\]

in which:

- \(\text{PEC}_i\) = average homogeneous water concentration in zone i (g.m\(^{-3}\))
- \(L_i\) = total load in zone i (g.d\(^{-1}\))
- \(F_{r_{ij}}\) = average mass fraction of emission source j in zone i (-)
- \(E_j\) = emission of source j (g.d\(^{-1}\))
- \(T_i\) = average hydraulic residence time of zone i (d)
- \(V_i\) = average water volume of zone i (m\(^3\))
- \(n\) = number of emission sources

Emission sources are river discharges, prefixed emissions in North Sea zones and atmospheric deposition. The mass fractions of emission sources in the North Sea were derived from calculations based on the North Sea Atlas (Ruijter and Postma, 1987). Applying these mass fractions, loss processes like volatilization, decay and settling are not considered. This is in line with a worst case approach, as it leads to overestimation of the probable exposure concentration.

The calculated probable exposure concentration for each North Sea zone and for each season are compared with the user-specified NEC value. In order to account for uncertainty in the estimated PEC due to ignoring actual concentration gradients, a safety factor (SF) is defined. The safety factor is set to 5, a number representative for the various North Sea zones, which was deducted from previous modelling studies.
The procedure distinguishes the following three possible conditions for each season:

1. \( \text{PEC}_i < 0.01 \text{ NEC/Sf} \) in all North Sea zones:
   
   Risks are not expected. There is no need to continue the computations.

2. \( 0.01 \text{ NEC/Sf} < \text{PEC}_i < 0.01 \text{ NEC} \) in one or more North Sea zones:
   
   A small but significant risk might occur for one or more North Sea zones. It is recommended to continue the computation.

3. \( \text{PEC} > 0.01 \text{ NEC} \) in one or more North Sea zones:
   
   Significant risks are likely to occur. Continue the computation.

**Physico-chemical substance characteristics**

The substance specific parameters are:

- molecular mass;
- partition coefficients; \( K_{oc} \), BCF, \( X_{doc} \) and/or \( K_{ow} \) for organic micropollutants;
- Proton dissociation constant;
- Henry’s constant at 20°C;
- saturated vapour pressure at 20°C;
- aqueous solubility at 20°C;
- melting temperature; and
- degradation rates at 20°C; \( r_w \), \( r_s \), and \( k_{oth} \); different values for a drainage system, a river and the North Sea.

The programme demands the most probable and worst case value of most parameters. Data for these parameters, or even for basic physical and chemical properties will appear unavailable for many chemicals, especially for new organic chemicals being considered for bulk manufacture. However, a wide variety of methods exist in chemistry (and toxicology) to estimate the above environmental process parameters (and toxic effect concentrations). An important limitation of the applicability of these methods, commonly called "Quantitative Structure-Activity Relationships" (QSARs), is that relationships can only be established, and subsequently used as prediction tool, for compounds with a common mode of physio-chemical behaviour or reactivity.

A review of environmental fate models, hazard ranking schemes, governmental regulations and other material first led to the identification of about 50 physio-chemical properties of interest. Only a few properties, however, control most of the variability in environmental behaviour, and are therefore shared by all transport modules in water quality models. One of the most important parameters that explains the fate of chemicals in the aquatic environment is the water solubility or better, the aqueous activity coefficient.
Highly soluble chemicals are easily and quickly distributed in the hydrological cycle. These chemicals tend to have relatively low adsorption coefficients for soils and sediments and relatively low concentrations in aquatic biota. They also tend to be more readily biodegradable by microorganisms in surface waters and water treatment plants. The rates of other degradation processes (e.g., photolysis, hydrolysis, and oxidation) and specific transport processes (e.g., volatilization and washout from the atmosphere by rain) are also affected by the extent of water solubility. Therefore, this parameter or related parameters, such as the octanol-water partition coefficient \( K_{ow} \), can be used to estimate the parameters that determine the fate of micropollutants in natural systems.

The following QSARs have been selected for SCREMOTOX:

- **Octanol-water partition coefficient** \( K_{ow} \) (Isnard and Lambert, 1989)

  For \( T_m < 25 \, ^\circ C \):
  \[
  \log K_{ow} = 4.62 - 0.72 \log(1000 \, S_w)
  \]
  (3.42)

  For \( T_m > 25 \, ^\circ C \):
  \[
  \log K_{ow} = 4.81 - 0.77 [\log(1000 \, S_w) + T_m - 25]
  \]

  \( T_m \) is the melting temperature (°C).

- **Aqueous solubility** \( S_w \) (Isnard and Lambert, 1989)

  \[
  \log S_w = -1.62 \log K_{ow} + 1.0 - 0.0054 (T_m - 25)
  \]
  (3.43)

  Melting temperature \( T_m \) is set to 25 °C for liquid compounds.

- **Henry’s Law constant** \( H \)

  \[
  H = M_w.P_v/S_w
  \]
  (3.44)

  \( M_w \) is the molecular weight.

  \( P_v \) is the saturated vapour pressure at 20 °C.

- **Partition coefficient** \( K_{oc} \)

  \[
  K_{oc} = K_{ow} \cdot f_{ad}
  \]
  (3.45)

  \( f_{ad} \) is the non-dissociated fraction, calculated from \( 1/[10^{(pH-K_a)} + 1] \).

  \( K_a \) is the equilibrium constant for the acid dissociation reaction.

  The pH is given an average value (8).

These SARs are recommended for application at the stage of initial risk screening of aquatic pollutants with missing (experimental) information on environmental fate parameters. They have been selected on features such as state of validation, statistical quality and availability in databases.
Effect concentrations

The substance specific effect concentrations, also called test values, concern the NEC and the EC_{50} for three exposure-effect routes, respectively water, (suspended) sediment and food. The determination of the test values, such as the NEC, proceeds by means of extrapolation from experimental ecotoxicological data. In recent years a number of methods have been developed for this purpose. See section 3.5.2 for the OECD method that has been adopted for SCREMOTOX. In this method, the lowest available (and acceptable) value is selected and an empirical safety factor is applied to this value, varying from 10 to 1000. The magnitude of the safety factor depends on the type of data (chronic NOEC or acute EC_{50}) and the representativeness of the data for target organisms, such as algae, crustaceans or fish.

Emissions

The emission loads are estimated according to the USES-methodology (section 3.1) or are directly provided by the user on the basis of unequivocal data. The estimation method requires:

- quantities of production, import and export;
- emission factors for five life cycle stages as functions of use categories, the solubility and the octanol-water partition coefficient;
- retention factors for sewage treatment plants; and
- land use factors for river basins and countries.

Tables to determine the emission factors, retention factors and land use factors (Rhine river basin) are included in Appendix A. These factors are part of the prefixed input.

A third option is the imposing of 'observed' loads in stead of 'estimated' loads in rivers. This option demands for observed concentrations and, depending on the calculation method used, measured flow rates.

Parameters concerning transport and retention

The prefixed, mostly compartment specific input concerns:

- water-air transfer coefficients k_w and k_a;
- settling rate S_s;
- partial flushing ratios: flush_i (in fact seasonally average flow rates);
- physical properties: volumes V_w and V_s, surface areas A and A_s;
- compositional properties: concentrations of suspended matter, phytoplankton and DOC; organic fractions f_{org} in suspended matter and sediment, sediment fraction f_{sed}.
- reference (heavy metal) deposition fractions for each country; and
- travel distances between for each combination of country and zone.

The fact that water-air transfer coefficients are slightly substance specific is ignored. The present version of SCREMOTOX has prefixed compartment specific values. The other parameters are season specific, except for the physical properties. Four sets of tables are available, one for each season.
3.7 Output

The output consists of logical and numerical information. The logical information concerns questions and options put forward to the user by the question-decision procedure to guide him through the computation. The numerical results of the computation are delivered for individual North Sea zones. The compartment and season specific output encompasses:

- expected mean and 95-percentile concentrations (total, particulate, in biota, dissolved) in the water column and in the sediment;
- worst case concentrations related to the uncertainty in substance characteristics;
- ecotoxicological risks, e.g. ratio's of exposure concentrations (PEC) and test values (effect concentrations such as NEC); the PEC/NEC ratio is an indicator for the chance of violation of test values;
- a risk class number for the computed case (combination of substance properties and emissions);
- the direct, upstream and atmospheric loads;
- percentual contributions of the sources to the loads; and
- retention and loss factors.

North Sea zones are ranked for the risk. The output concerning the mass balance is not ranked, but given in a prefixed order of compartments.

The output is presented in the form of:

- North Sea maps (total concentration, fractional concentrations and risks);
- tables ranked for North Sea zones and seasons (risks, concentrations, uncertainty, variability); and
- non-ranked tables per North Sea zone and per seasons (loads, percentual contributions in load).
4 Discussion, conclusions and recommendations

General

The present version of SCREMOTOX matches the methodological design (Waterloopkundig Laboratorium et al., 1995) to a large extent. Some extensions were made as this appeared necessary for achieving optimal results for risk assessment. Some aspects had to be dealt with in a less detailed way, as the constraints to the project did not allow further elaboration. Improvements to meet the specifications of the methodological design and other improvements are discussed briefly below.

It appeared to be impossible to make a fully operational version of SCREMOTOX within the constraints of the project. It is not operational in the sense that it can be used already for the actual screening of substances. However, the software functions adequately from a technical point of view. SCREMOTOX has yet to be supplied with values for the physical and water quality parameters of the river basins. Tentative values have only been implemented for the Rhine River basin in order to facilitate testing of the program.

When SCREMOTOX has been provided with appropriate river-specific data, it is to be validated by means of application/calibration on the data for two well-known substances. These substances have to differ distinctly with respect to their properties, especially with respect to partitioning.

Moreover, the functionality and user friendliness of SCREMOTOX should be tried by a group of users, which may be done adequately in the form of a workshop focussing on risk assessment for a number of poorly known substances. Improvements and/or extensions may have to be made depending on the findings of such a workshop.

Emission

The module for estimation of the emissions strongly relies on a worst case approach, which may lead to substantial overestimation. Elaboration of the module taking into account more details of the USES methodology such as a further break down of the emission factors according to use categories should be scrutinized. Incorporation of the tables containing the emission factors in the software is to be considered.

Transport and retention in the river basin

The behaviour of a micropollutant in the compartments of a river basin is described with exactly the same formulations for each compartment. It is doubtful whether the formulations are adequate for the estuarine compartment in case of a stratified estuary. The formulations need to be evaluated and, if necessary, to be improved for this compartment. However, selecting appropriate values for the physical parameters may counteract the shortcomings of the formulations substantially.
Transport and retention in the North Sea

SCREMOTOX uses only one steady state hydrodynamical flow field for the transportation of water and substances in the North Sea. This flow field represents approximately the residual flow field for long term average conditions (yearly average discharge of river basins and representative wind field). However, the conditions may vary substantially among the seasons. Therefore, it is recommended to implement seasonally average flow fields in SCREMOTOX. Such flow fields relate to the wind fields and river discharges that are representative for seasons.

Atmospheric deposition

SCREMOTOX considers the atmospheric deposition of organic substances on the basis of the overall, mainly aerosol-borne deposition flux of heavy metals. A systematic distinction of the various forms of dry and wet deposition, leading to a more substance-specific approach, is not made. It seems that it is feasible to consider more detail within this respect, starting from partitioning among the gaseous and aerosol fractions. A formulation for the partitioning is already available. Considering dry deposition explicitly will allow coupling with volatilization from the water column, which is ignored presently.

The atmospheric deposition and the coupling of deposition and volatilization in river basins have also been ignored. It is thought that these processes contribute only slightly to the loading of the North Sea, as the surface water system covers only a few percent of the river basin area and volatilization is usually a minor sink. Nevertheless, a well argued execution for this has yet to be developed.

Moreover, improvement is possible with respect to the calculation of travel times between a country and a North Sea zone. Linear distances are taken, whereas correction factors for non-linearity of trajectories are required.

The uncertainty range of the calculated atmospheric deposition flux can not yet be estimated. Rules of thumb to quantify ranges are badly needed, as the quantification of the ranges will allow better determination of the worst case deposition flux.

Exposure concentrations

The exposure concentrations in (suspended) sediment are given as absolute values. The particulate concentrations in the North Sea refer to settling or recently settled, fine cohesive sediment. This implies that a direct comparison with sediment quality standards is impossible. Comparison with the Dutch standards requires a step-wise conversion of the concentrations. The first step involves conversion into the overall actual concentration in the sediment using the sand fraction. These concentrations are converted to normalized concentrations relative to the actual organic matter fraction (and the < 2μm particle fraction in case of heavy metals) in the second step. These conversions and the required normalization formulations should be made part of SCREMOTOX.
Ecotoxicological risk

Considering the dominant role of NEC-values in risk assessment, it is of major importance that best guess estimates are produced next to worst-case values, if experimental data are very scarce or lacking. QSAR’s are available for this purpose in the qsar System programme, which is operational with rikz, riza and rivm. A procedure for using QSAR’s should be made part of the SCREMOTOX methodology. Methods for the determination of NEC’s and EC_{50}’s should be incorporated in the software as much as possible.

The PEC/NEC-computation should take into account, that dependent on the properties of a substance elevated concentrations may occur in the 'micro surface layer'. An enhanced risk factor might be introduced in a future version of SCREMOTOX for this purpose. Considering the concentrations in the micro surface layer explicitly does not seem to be required.

Functionality of the SCREMOTOX program

Functionality may be enhanced with respect to:

- tracking down of important causes of uncertainty in the predicted exposure concentrations (substance-specific parameters and emissions) by means of quantification of the percentual contributions of the causes in the uncertainty bands of these concentrations;
- quantification of natural variability taking into account fluctuations of emissions, river discharges and North Sea flow fields next to spatial differences in North Sea zones;
- the execution of computations only if they are meaningful considering both the accuracy of the simulation and the expected risks;
- extension of the formulations to make them also suitable for heavy metals (this requires minor changes);
- connection to data-bases, for instance data-bases for substance-specific parameters (experimental data and QSAR’s) and for emission data in order to provide default values and basic data; and
- integral analysis of the risks of groups of substances.

Improving quantitative insight into uncertainty and natural variability will allow a better defined worst case approach and will help setting priorities with respect to the production of research and field data for individual substances.

The present version of SCREMOTOX estimates the expected maximal exposure concentrations in the North Sea at the point where all riverine loads have been determined. The program suggests the user to abandon further computations when these concentrations do not create risks. A similar procedure could be developed for the earlier stage of emission calculation.

It should also be possible to predict the accuracy of the exposure concentrations at several stages of the computations. Dependent on the expected accuracy and criteria for acceptable inaccuracy, the user may be recommended to refine the input or, even better, to start the collection/production of more accurate data. An interactive procedure to reduce inaccuracy and to determine priorities for data collection by means of research and monitoring should be worked out in more detail.
Performance of the SCREMOTOX program

The performance of the SCREMOTOX program may be improved in various ways. The REXX-based interface does not provide facilities for implementation of an automated question-decision procedure, that takes the user along the computations depending on the decisions that are made. So instead of automated guiding, the program produces information to help the user through the input procedure and the computations, but the user always decides which action is to be taken next. Most of the information has been incorporated in menus. Some comments appear on the screen after completion of a part of the computation. Future applications (probably operating under WINDOWS) can be improved in the sense that the user is guided in more detail and in a more unequivocal way.

The user interface can be made much more supportive. Selections made with respect to compartments and seasons should in future versions affect the content of screens in the sense that lists of compartments are reduced and that input for nonselected seasons is blocked. Moreover, the present version does not allow the user to overrule the emission distribution among countries, river basins and compartments produced by the emission estimation module. However, it may well be that the user has specific information on this distribution that is conflicting with the calculated distribution. It would therefore be an improvement when an option is added for user defined redistribution, although manipulation is already possible to a certain extent when the option of 'prefixed emissions' is used.

Several procedures to determine input to SCREMOTOX are provided in the present report, but have not or only partially been integrated in the software and its interface. The procedures for determination of the substance-specific parameters, the emission factors and the effect concentrations (NEC, EC₉₀) have not been included at all. The input of river basin properties can only be done by direct editing of input files. It seems that substantial extra support will be given to the user, when bigger parts of these procedures and the required data are incorporated in the software of SCREMOTOX and when river basin properties can be inserted in interface menus.

Another aspect of performance that needs improvement concerns graphical and tabular output. Future versions of SCREMOTOX should be extended with more graphical output facilities next to the existing tabular output, such as rankings, time series, bar diagrams, etc. Additional ways of ranking of North Sea zones may be considered, in particular with respect to concentrations. Hardcopies of the output must be made directly available to the user through the addition of reporting facilities to the user interface.
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Part II: Concise user’s manual (version 1.00)
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1 Introduction

The computer program of SCREMOTOX is operated through a user interface program. The interface has been structured according to question-decision procedures. The reasons for this have been explained in part I of this report. The main objective of these procedures is to minimize undefined uncertainty and inaccuracy in the input for SCREMOTOX.

The present version of the interface focuses on composing of the input for SCREMOTOX. The output can be partially viewed through the interface. However, all output is stored in files, containing tabelized data. The comments given by the program to help the user composing optimal input and running the computational subprograms in a meaningful way are not yet very extensive. Improvement of the interface and extension of the output facilities should have the highest priority at the construction of improved versions of SCREMOTOX.

Chapter 2 offers information on how to quantify the substance specific input with respect to process parameters and emission factors (see also Appendix A). Chapter 3 describes the main structure of the user interface. The input procedures are dealt with in chapter 4. The facilities for execution of subprograms and for viewing of output are illuminated in chapter 5. General software and hardware requirements can be found in chapter 6.
2 Composing the input of SCREMOTOX

The input that the user will provide to SCREMOTOX will be inaccurate to a certain extent, which leads to uncertainty in the results of the computations. The formulations of the computational procedures are an additional source of uncertainty, as they describe a simplified representation of the real world. The user should control the uncertainty as much as possible. Suggestions for composing optimal input and critical remarks on the procedures are provided in the next sections with respect to substance characteristics and emissions.

2.1 Physico-chemical substance property quantification

2.1.1 General considerations

Values for substance specific environmental fate parameters to be used in SCREMOTOX should be selected from data sources in a systematic way in order to minimize undefined inaccuracy. This procedure involves the scanning of data sources in a prescribed order according to a question-decision procedure. When it turns out that data are lacking for a specific parameter, structure-activity relationships (SAR’s) can be used to estimate a value. A default value may be used when appropriate SAR’s are not available.

For new substances that will be imported or commercialized in the Netherlands, the European Community base set for new chemicals has to be provided. This includes aqueous solubility, n-octanol/water partition coefficient and the vapour pressure. For existing chemicals an extensive data set on environmental chemical properties according to HEDSET (the ECOECD Harmonized Electronic Data Set for existing chemicals) is required from companies who intend to market a substance. The properties include Henry’s constant, the solubilities in water and fat, the vapour pressure, the octanol/water partition coefficient, the sediment/water partition coefficient and the degradation rates in soil/sediment and in water (RIVM, 1994).

Premanufacturing notification of chemicals, however, is less demanding (RIVM, 1994). Ecotoxicological data and most environmental fate parameters are not required for technical or scientific reasons (Vermeire et al., 1993). If not available, they will have to be estimated using SAR’s. To verify claims of companies which intend to situate or change chemical production facilities alongside Dutch rivers and estuaries under the 1970 Pollution of Surface Water Act, water quality authorities need this information for initial risk assessment (the screening stage).

Two values have to be provided to SCREMOTOX for a specific environmental fate parameter, the most probable (preferential) value and the worst case value. The probable value is defined as the best (average) value, measured or estimated for appropriate environmental conditions.
For details see the AQUAPOL database report (WL and MTC, 1995). The worst case in terms of ecotoxicological risk is generally related to slow degradation (biodegradation, photo-oxidation, etc.), slow volatilization and high organic matter/lipid affinity ($K_{ow}$, BCF), implying low aqueous solubility and low vapour pressure. However, the situation is more complicated when considering the North Sea. High partition coefficients lead to strong adsorption to suspended solids, to relatively high retention in fresh surface water, and hence to minimal pollutant discharges into the North Sea. As a compromise, SCREMOTOX demands low estimates for the partition coefficients and a high estimate for the bioconcentration factor (BCF) in the worst case computation.

The SAR’s incorporated in SCREMOTOX are described in section 3.6 of part I. The use of these SAR’s is recommended for application at the stage of initial risk screening of aquatic pollutants with missing (experimental) information on environmental fate parameters. The SAR’s have been selected on features such as state of validation, statistical quality, operational at and available from Dutch institutes (WL, RIKZ, RIZA, TNO and RIVM), and the possibility of automated calculation. Most recommended SAR’s are incorporated in the QSAR System program of the Montana State University and the Environmental Protection Agency at Duluth (QSAR System, 1986), which is operational at RIKZ and RIZA, just like the MedChem software (1989). QSAR System requires the Chemical Abstract Service (CAS) number or the SMILES string (Simplified Molecular Identification and Line Entry System; a linear representation of 2D and 3D molecular structures) of the substance considered as input. More advanced SAR methods, such as Linear Solvation Energy Relationships of solvatochromic parameters (LSERS), solubility parameter models (SOLPAR), UNIFAC methods (UNIQUAC Functional group Activity Coefficient) and the molecular connectivity indices method (MCI) are not yet generally applicable (Evers et al., 1990), and are therefore not discussed here.

### 2.2.2 Octanol-water partition coefficient

The octanol-water partition coefficient ($K_{ow}$) is a key parameter in studies of the environmental fate of organic chemicals, representing the tendency of chemicals to distribute between aqueous and organic (lipid) phases (Lyman et al., 1990). It has been found to be related to water solubility, soil-sediment adsorption coefficients and bioconcentration factors for aquatic life. Because of its increasing use in the estimation of these properties, the estimation of $K_{ow}$ is of crucial importance in exposure assessment (OECD, 1993). If no reliable experimental data are available, several SAR methods can be applied to estimate the value of $K_{ow}$. The most frequently applied and recommended procedure is the fragment constant method by Hansch and Leo (1979) which is used in the MedChem software (1989). The log $K_{ow}$ is calculated from essential group fragment constants and structural factors, including different bond types such as double bonds or conjugated double bonds and factors for geometrical properties, for example rings or chains.
The basic steps of property estimation are:

(1) Is log $K_{ow}$ value available from product information?

Yes: Use this value in the calculations and apply an uncertainty range of 0.04 log $K_{ow}$. The lower limit of this range can be regarded as a worst case. No: Continue.

(2) Is an experimental log $K_{ow}$ value available from the following databases:
- AQUAPOL (select the most relevant environmental conditions);
- MACKAY et al., 1992a and 1992b;
- other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.04 log $K_{ow}$. The lower limit of this range can be regarded as a worst case. No: Continue.

(3) Is a SAR log $K_{ow}$ value available from the following databases:
- AQUAPOL (select the most relevant environmental conditions);
- MACKAY et al., 1992a and 1992b;
- other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.1 log $K_{ow}$. The lower limit of this range can be regarded as a worst case. No: Continue.

(4) Can log $K_{ow}$ be calculated with the MedChem-ClogP program? (Input: CAS-number or SMILES string, see Verhaar and Hermens, 1992).

Yes: Use this value in the calculations and apply an uncertainty range of 0.1 log $K_{ow}$. The lower limit of this range can be regarded as a worst case. No: Continue.

(5) Is a value for the solubility ($S_w$) given?

Yes: Derive $K_{ow}$ from the solubility according to the following relationship considering the melting temperature (Isnard and Lambert, 1989; see section 3.6 of part I). Use this value in the calculations and apply an uncertainty range of 0.2 log $K_{ow}$. The lower limit of this range can be regarded as a worst case. No: Give an expert guess and apply a range of at least 0.5 log $K_{ow}$. The lower limit of this range can be regarded as a worst case.
2.2.3 Aqueous solubility

The water solubility ($S_w$) of a compound can be used, together with the vapour pressure, to calculate Henry's constant. If no reliable experimental data are available, several SAR methods can be applied to estimate the value of $S_w$. For liquid compounds, water solubility is highly correlated with the $K_{ow}$. The qsar System program uses a linear correlation with the log $K_{ow}$ value and is dependent on the temperature.

The basic steps of property estimation are:

(1) Is $S_w$ value available from product information?

Yes: Use this value in the calculations and apply an uncertainty range of 0.05 log $S_w$. The lower limit of this range can be regarded as a worst case.
No: Continue.

(2) Is an experimental $S_w$ value available from the following databases:
- AQUAPOL (select the most relevant environmental conditions);
- MACKAY et al., 1992a and 1992b;
- other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.05 log $S_w$. The lower limit of this range can be regarded as a worst case.
No: Continue.

(3) Is a SAR $S_w$ value available from the following databases:
- AQUAPOL (select the most relevant environmental conditions);
- MACKAY et al., 1992a and 1992b;
- other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.1 log $S_w$. The lower limit of this range can be regarded as a worst case.
No: Continue.

(4) Can $S_w$ be calculated with the qsar System program? (Input: CAS-number or SMILES string, see Verhaar and Hermens, 1992).

Yes: Use this value in the calculations and apply an uncertainty range of 0.1 log $S_w$. The lower limit of this range can be regarded as a worst case.
No: Continue.

(5) When no reliable compound class specific qsar is available, an equation is given by Isnard and Lambert (1989), which is based on a large database of "mixed" chemicals (n=300). See section 3.6 of part I.
Can $S_w$ be calculated with this equation?

Yes: Use this value in the calculations and apply an uncertainty range of 0.2 log $S_w$. The lower limit of this range can be regarded as a worst case.
No: Give an expert guess and apply a range of at least 0.5 log $S_w$. The lower limit of this range can be regarded as a worst case.
2.2.4 Vapour pressure

The vapour pressure ($P_v$) of organic substances is an important parameter in prediction the behaviour and fate of chemicals introduced into the environment. Estimated $P_v$ values may be subjected to considerable uncertainty, especially when no experimental boiling point is used but a "Meissner estimation". The uncertainty is of major importance when the calculated value is used together with $S_m$, calculated from log $K_{ow}$ to estimate Henry’s constant.

(1) Is the $P_v$ value available from product information?

Yes: Use this value in the calculations and apply an uncertainty range of 0.05 log $P_v$. The lower limit of this range can be regarded as a worst case.
No: Continue.

(2) Is an experimental $P_v$ value available from the following databases:
- AQUAPOL (select the most relevant environmental conditions);
- MACKAY et al., 1992a and 1992b;
- other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.05 log $P_v$. The lower limit of this range can be regarded as a worst case.
No: Continue.

(3) Is a SAR $P_v$ value available from the following databases:
- AQUAPOL (select the most relevant environmental conditions);
- MACKAY et al., 1992a and 1992b;
- other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.1 log $P_v$. The lower limit of this range can be regarded as a worst case.
No: Continue.

(4) Is an experimental boiling point (°K) available? (Input: CAS-number or SMILES string - see Verhaar and Hermens, 1992 - and an experimental boiling point.)

Can $P_v$ be calculated with the QSAR System program?

Yes: Calculate $P_v$ with the QSAR System program, use this value in the calculations and apply an uncertainty range of 0.2*log $P_v$. The lower limit of this range can be regarded as a worst case.
No: Give an expert guess and apply a range of at least 0.5 log $P_v$. The lower limit of this range can be regarded as a worst case.
2.2.5 Henry’s constant

Henry’s constant (H) describes the partitioning of a chemical between air and water. For substances with low water solubility (<1.0 mol/l) Henry’s constant can be calculated from water solubility and vapour pressure. This method is used by the QSAR System program. If calculated P_v and S_w values are used to estimate H, the respective uncertainties have to be considered.

(1) Is the H value available from product information?

   Yes: Use this value in the calculations and apply an uncertainty range of 0.05 H. The lower limit of this range can be regarded as a worst case.
   No: Continue.

(2) Is an experimental H value available from the following databases:
   - AQUAPOL (select the most relevant environmental conditions);
   - MACKAY et al., 1992a and 1992b;
   - other?

   Yes: Use this value in the calculations and apply an uncertainty range of 0.05 H. The lower limit of this range can be regarded as a worst case.
   No: Continue.

(3) Is an SAR H value available from the following databases:
   - AQUAPOL (select the most relevant environmental conditions);
   - MACKAY et al., 1992a and 1992b;
   - other?

   Yes: Use this value in the calculations and apply an uncertainty range of 0.1 H. The lower limit of this range can be regarded as a worst case.
   No: Continue.

(4) Can H be calculated with the QSAR System program?

   Yes: Use this value in the calculations and apply an uncertainty range of 0.2 H. The lower limit of this range can be regarded as a worst case.
   No: Use a default value of 0 (no volatilization).
2.2.6 Sediment-water partition coefficient

Sorption coefficients reflect processes of distribution of a compound to the major solid and dissolved organic matrices in the water column such as suspended matter, sediment and dissolved organic matter. These distribution coefficients are influenced by temperature, salinity, pH and sediment type. Normalizing the distribution coefficients to an organic carbon basis reduces the variance of sorption coefficients measured in different soils for hydrophobic chemicals to one order of magnitude (Karickhoff, 1984; DiToro et al. 1991), but for more polar chemicals the normalized $K_{oc}$ values may still vary by a factor of 100-1000. For predicting sorption coefficients various descriptors such as log $K_{oc}$, $S_w$, molar refraction and connectivity indices have been used. Gerstl (1990) gives equations for log $K_{oc}$ as function of log $K_{oc}$ for 16 defined series of compounds, that are based on a large database. The equations are listed in Bockting et al., 1993.

(1) Is the $K_{oc}$ value available from product information?

Yes: Use this value in the calculations and apply an uncertainty range of 0.05 log $K_{oc}$. The upper limit of this range can be regarded as a worst case.
No: Continue.

(2) Is an experimental $K_{oc}$ value available from the following databases:
   - AQUAPOL (select the most relevant environmental conditions);
   - MACKAY et al., 1992a and 1992b;
   - Gerstl, 1990;
   - MedChem program;
   - other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.05 log $K_{oc}$. The upper limit of this range can be regarded as a worst case.
No: Continue.

(3) Does the compound contain acidic groups (e.g., hydroxyl or carboxyl groups)?

Yes: Take the acid dissociation (pKa) into account from the MedChem-Thor database or calculated with the QSAR System program. The MedChem software provide access to the Thor database containing partition coefficients and pKa values. Assuming only sorption of the parent acid the $K_{oc}$ can be corrected according to the equation described in part I, section 3.6.
Use this value in the calculations and apply an uncertainty range of 0.1 log $K_{oc}$. The upper limit of this range can be regarded as a worst case.
No: Continue.
(4) Is an SAR $K_{oc}$ value available from the following databases:
   - AQUAPOL (select the most relevant environmental conditions);
   - MACKAY et al., 1992a and 1992b;
   - other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.2 log $K_{oc}$. The upper limit of this range can be regarded as a worst case.
No: Continue.

(5) Can log $K_{oc}$ be calculated with the QSAR System program?

Yes: Use this value in the calculations and apply an uncertainty range of 0.2 log $K_{oc}$. The upper limit of this range can be regarded as a worst case.
No: Take $K_{oc} = K_{ow}$ and apply an uncertainty range of 0.5 log $K_{oc}$. The upper limit of this range can be regarded as a worst case.

2.2.7 Bioconcentration factor in fish

The bioconcentration factor (BCF) of non-ionic organic chemicals in fish can be described as an equilibrium between water and fat, dependent on the hydrophobicity of the chemical ($\log K_{ow}$). The correlation between BCF and Kow will be linear as long as the ratio of the respective activity coefficients remains constant (predictor in SCREAMOTOX is BCF = $K_{ow}$). Predominantly due to variable experimental conditions deviations and apparent loss of linearity occurs frequently, especially for superlipophilic compounds. If a reliable measured value is not available, the estimation method according to Veith and Kosian (1983), which is used in the QSAR System program, can be applied. A worst case estimate of bioconcentration has been postulated by Nendza (1991), who suggested a nonlinear function based on $\log K_{ow}$ describing the highest log BCF associated with a given hydrophobicity, which corresponds to the bioconcentration potential of a chemical. If discrepancies between measured and calculated values then occur, the measured BCFs are lower than calculated.

(1) Is BCF value available from product information?

Yes: Use this value in the calculations and apply an uncertainty range of 0.05 log BCF. The upper limit of this range can be regarded as a worst case.
No: Continue.

(2) Is an experimental BCF value available from the following databases:
   - AQUAPOL (select the most relevant environmental conditions);
   - MACKAY et al., 1992a and 1992b;
   - other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.05 log BCF. The upper limit of this range can be regarded as a worst case.
No: Continue.
(3) Is a SAR BCF value available from the following databases:
- AQUAPOL (select the most relevant environmental conditions);
- MACKAY et al., 1992a and 1992b;
- other?

Yes: Use this value in the calculations and apply an uncertainty range of 0.1 log BCF. The upper limit of this range can be regarded as a worst case. No: continue.

(4) Can BCF be calculated with the QSAR System program? According to the equation of Veith and Kosian (1983):
\[ \log \text{BCF} = 0.79 \log K_{ow} - 0.4 \]

Yes: Use this value in the calculations and calculate a worst case value with the bilinear model of Nendza (1991):
\[ \log \text{BCF} = 0.99 \log K_{ow} - 1.47 \log (4.97 \times 10^4 K_{ow} + 1) + 0.0135. \]

2.2.8 Degradation rate constants

Four major categories of biodegradable chemicals are distinguished considering their potential for persistence and accumulation in the environment. These categories define in quantitative terms many of the qualitative descriptions of (bio)degradability that currently permeate environmental decision-making and regulatory assessments. Anaerobic biodegradation in sediment is generally a very slow degradation process for which good estimates are not available usually. No biodegradation may be used as an absolute worst case condition.

Other routes of degradation, such as hydrolysis and photolysis can be important for certain classes of compounds; e.g alkyl halides, amines, carbamates, ester, epoxides and nitriles (Lyman, 1989). QSAR System provides a very rough estimate of these degradation routes and half-life times, which can be used when specific data are not available. The steps that should be followed are similar to steps necessary for the estimation of the biodegradation half-life mentioned below. It is recommended to use the summed value of all degradation half-life times as input value for SCREMOTOX.

First-order degradation kinetics with rate k is assumed. This means that the rate of biodegradation is directly proportional to the concentration of the substance. The ratio of the biodegradation half-life (T_{0.5}) and the residence time can be used for classification. T_{0.5} can be calculated from the relationship \( T_{0.5} = \ln 2/k \). Assuming typical residence times of 10 days of compounds in SCREMOTOX compartments, the following four categories are distinguished (Larson and Cowan, 1995):

1. Readily biodegradable; These substances do not accumulate or persist in the environment. Their T_{0.5} in SCREMOTOX compartments is generally less than 1 day.
2. Practically biodegradable; These substances reach steady-state levels quickly in the environment. Once input has stopped, practically biodegradable compounds do not accumulate or persist. Their T_{0.5} is generally more than 5 days and less than 20 days.
3. Slowly biodegradable; These substances accumulate as a function of their usage and removal rates, and they can persist for extended periods of time after their use has been discontinued. Slowly biodegradable chemicals will not persist indefinitely, since finite rates of degradation do occur. They have significant potential to accumulate and persist in the environment, if other physicochemical removal mechanisms are not present. Their $T_{0.5}$ is generally more than 20 days and less than 50 days.

4. Nonbiodegradable; These substances show little if any evidence of significant mineralization by environmentally realistic assemblages of microorganisms. They accumulate as a direct function of their usage, and they do not reach equilibrium or steady state levels. Nonbiodegradable chemicals persist more or less indefinitely in the environment after their input has been stopped at levels defined by their loading rate and duration of use. Their $T_{0.5}$ is much longer than 50 days.

The QSAR System program uses a principal component analysis of 16121 BOD5 tests of 287 compounds in which molecular size and specific structural features determine more than 94% of the variance (Niemi et al., 1987).

The following procedure is recommended to determine the biodegradation half-life of substances under aerobic conditions (water column and upper mm's of the sediment):

1. Are a $T_{0.5}$ value or terms such as readily, practically, slowly or nonbiodegradable available from product information?

   Yes: Use this value or the above mentioned classification values in the calculations, and apply an uncertainty range of 0.1 $T_{0.5}$. The worst case value can be taken 100 days.
   No: Continue.

2. Is a specific (experimental) $T_{0.5}$ value available from the following databases:
   - AQUAPOL (select the most relevant environmental conditions);
   - MACKAY et al., 1992a and 1992b;
   - other?

   Yes: Use this value in the calculations and apply an uncertainty range of 0.1 $T_{0.5}$. The worst case value can be taken 100 days.
   No: Continue.

3. Is a SAR $T_{0.5}$ value available from the following databases:
   - AQUAPOL (select the most relevant environmental conditions);
   - MACKAY et al., 1992a and 1992b;
   - other?

   Yes: Use this value in the calculations and apply an uncertainty range of 0.1 $T_{0.5}$. The worst case value can be taken 100 days.
   No: Continue.
(4) Can T_{0.5} be calculated with the QSAR System program? (Input: CAS-number or SMILES string; see Verhaar and Hermens, 1992.)

Yes: Use this value in the calculations and apply an uncertainty range of 0.1 T_{0.5}. The worst case value can be taken 100 days.
No: Take an absolute worst case value T_{0.5} is 1000 days.

2.2 The emission estimation module

The emission module is described in section 3.1.1 of part I. Errors in the estimation of the emissions in river basins occur mainly at the following stages:

- quantification of overall production, import and export (input);
- estimation of the overall emissions (computation); and
- spatial distribution of the overall emissions (computation).

Production, import and export

Although EC-data for the whole of the EC-countries or for subsets of these countries are probably the most accurate data available, it is obvious that quite a few 'best possible' guesses were made in composing these data. The user might consider applying his own safety factor to data, that are obtained from EC-databases.

Moreover, the USES-approach was designed for yearly average conditions, whereas emissions may not be evenly spread over the year at all. Application of agricultural chemicals is sometimes done only once a year. Chemicals are often produced batchwise a few times per year, especially when small volumes are involved. The real emissions may be concentrated in a short period of time. Yet, the time span of emission to the North Sea will be stretched by retention in the natural system.

Discharges into the environment at several (or numerous) locations will generally not take place simultaneously. Moreover, soil bound residues of agricultural chemicals will be eroded into local surface waters only at high rainfall events, taking place only a few times a year. And before that sometimes the residues are already mixed with less contaminated soil due to plowing. Retention in the surface water system will cause a further smoothing in time of emission to the North Sea.

Therefore, no large errors will be generated by taking a minimum timestep of three months. In case the user expects the emission to take place in mainly one season, he should make a worst case computation by assigning the whole yearly emission to that particular season.
Overall emissions

Uncertainties are generated by the emission factors, that have to be selected from the tables in Appendix A. However, a worst case approach was followed in composing those tables from the more detailed USES-methodology.

The emission factor for a class of chemicals (HEDSET classes and chemical properties) will never be exactly the same for all substances within that particular class but will vary around the estimated value. Assuming a log-normal distribution, the 95 % confidence interval lies between M/k and M.k; M and k being the 'Release' and 'Dispersion factor' from the tables in Appendix A (Slob, 1994). In general the uncertainty increases as the emission factor decreases. Dispersion factors lie between 1 and 5 for the highest factors and between 3 and 12 for the lowest ones. As an example the production plus import minus export of 1 ton of an industrial category 6 chemical (public domain) would give an estimated emission at the processing stage of 900 kg to waste water. With a dispersion factor of 1.1 the 95 % confidence interval than would lie between 820 and 990 kg.

Within every class of chemicals there can be substantial differences in emission due to the divergent uses or other differences between chemicals. In the USES emission module sometimes a sub division is made according to these specific uses or substance. This additional specification is left out for the sake of simplicity, bearing in mind the screening objective of this ranking system. From all possible values within one class of the USES emission module the highest one is taken as a worst case value. Consequently, considerable overestimation of the real emission is possible.

Compared to SCREMOTOX, further subdivisions are made in USES for the industrial categories 6 (public domain), 8 (metal extraction, refining and processing), 10 (photographic industry), 12 (pulp, paper and board industry) and 13 (textile processing industry) at the processing stage. For industrial category 6 a subdivision is made at the stage of private use and for industrial category 12 a subdivision is made at the stage of recovery (Jager and Visser, 1994).

Spatial distribution

The allocation of aggregate emissions for a group of countries to river basins is based on land use information. For diffuse sources this assumption does not lead to substantial errors, but especially for point sources this method can cause large uncertainties. Point sources can be located either inside or outside a river basin hence their allocation factor can only be 0 or 1. Yet, the model uses a factor based on urban land use between 0 and 1 to allocate the source to a specific river basin. In general this factor is a small number in the order of 0.1 (about 0.2 for the Rhine basin). The error connected with the allocation of one individual point source to one river basin can be substantial. Yet, the maximal 'geographic error' may have a low likelihood. The probability of a large error decreases with increasing number of sources. Household related emissions and the processing of agricultural chemicals are the most extreme cases.
The error in the geographical distribution may have a limited effect on the exposure concentrations when the error pertains to the discharges of adjacent river basins and when differences in retention in these river basins is small. A maximal effect will arise in case of incorrect distribution between the North Sea river basins and the other river basins in EC-countries. 61% of all urban area and 24% of all agricultural area lies inside the area draining into the North Sea. The user can counteract the consequences of incorrect geographical spreading of emissions by isolating 'well-known' areas of emission and imposing the connected emissions as 'prefixed' emissions in SCREMOTOX.
3 The user interface

The first screen appearing at the start of the program provides information on the name, the nature and the source of the software. The next screen, which appears automatically after some time, enables the user to run five subprograms from the main menu:

- Input (1)
- Emission (2)
- River basins (3)
- North Sea (4)
- Output (5)

Each of the subprograms can be entered, executed and terminated through pull-down menus. The subprograms have to be executed in the order as given on the screen. First, the user has to provide all substance- and case-specific input data, or has to make all modifications required to turn an existing case into the desired new case. The programs do not check whether these conditions have been obeyed!

In the present version of SCREMOTOX subprograms 2-5 have only a few pull-down menus, which enable the user to execute the program and to view output. After execution of a program a message may appear, containing suggestions on how to proceed. Subprogram 1 contains four input sections, which have to be passed through subsequentially. The sections are:

- Case information (1)
- Substance characteristics (2)
- Transport and retention (3)
- Emission data (4)

The data for sections 1, 2 and 4 are to be inserted in file independent menus. The data on transport and retention in river basins (flow rates, settling rates, phytoplankton concentration, etc.) are inserted through editing of the existing actual input files. A menu-driven input procedure to compose these files should replace direct editing in a future version of the software. The user may skip section 3 and use a standard setting for the North Sea system.

The input windows that appear may contain questions (yes/no), data input fields and comments. Generally, the fields are filled with values pertaining to the current case, that is the case of the previous session which may be the default case. If desired, the values may be overruled with default values during the session (press key F10). The files pertaining to the current case and the default case have fixed names and are the only files which are accessible for the program. If one wants to store the current case for future use, the user has to leave the interface, copy the current input files to another directory and rename them. If one wants to use another existing case than the previous one, these actions have to be carried out in reverse.

All screens contain explanation regarding the use of keys for operating the interface. The user may exit the interface at any stage by pressing 'Esc' repeatedly. The final screen that appears explicitly asks the user wether he wants to exit the program or not.
4 Input procedures

4.1 Case information

The first menu in this section should offer the possibility to define a completely new case or to attach files previously made for a specific case. The options in the menu read:

- Select existing case
- Create new case
- Provide substance name
- Select seasons
- Select compartments

The first two options have not yet been implemented. The screens appearing after invoking the options are mere examples of how cases may be selected or created in a future, more extended version of SCREMOTOX. The procedure for importing an existing case is described in chapter 3.

The substance name provided under the third option is stored in an input file of the current case and will appear in headers of output. The substance name of the current case is maintained if option three is not used.

The final two options are to be used for changing basic case information. This concerns the following:

a) For which seasons do you want to make calculations?

**Comments:**
The user may choose any combination of seasons. However, if the emission is mainly occurring in one season, it is recommended to select only this particular season. In all other cases, it is recommended to consider all seasons.

Select: (0=no/1=yes)

1 winter
1 spring
1 summer
1 autumn
b) Which river basins do you want to draw into the calculations?

**Comments:**
The user may choose any combination of river basins.

Select: (0 = no/1 = yes)

1  riverbasin A
1  riverbasin B
0   .....  
1  riverbasin N

c) Which countries do you want to impose/calculate emissions for?

**Comments:**
The user may choose any combination of countries.

Select: (0 = no/1 = yes)

1  country A
1  country B
0   .....  
1  country N

d) In which North Sea zones do you want to impose prefixed emissions?

**Comments:**
The user may choose any combination of zones.

Select: (0 = no/1 = yes)

1  zone A
1  zone B
0   .....  
0  zone N

The response of the subprogram is that it assigns the index 'yes' to selected seasons, river basins, countries and zones. The computational subprograms exclude the other seasons, countries and river basins from the simulation. This part of the interface is not yet effective regarding the remainder of the interface. That means that lists of compartments are not modified to include only the selected compartments. The four seasons are always displayed, even if only one has been selected. However, parameter values inserted for non-selected compartments and seasons are ignored by the subprograms. The interface of future versions of SCREMOTOX should be modified in such a way that it presents lists only containing selected compartments and seasons.
### 4.2 Substance characteristics

The first menu in this section divides the input parameters in two groups:

- Physical/chemical characteristics
- Ecotoxicological characteristics

The respective input menus read:

a) Supply data for the physical/chemical characteristics

**Comments:**
Supply values or let the program estimate values using a SAR (only for $K_{ow}$, $K_{oc}$, $S_{eq}$, $H$) by filling in -1. Physical/chemical values are to be selected according to the following preference:

1. Use product information
2. Use a database (AQUAPOL, MACKAY, other)
3. Use a SAR from a database (AQUAPOL, MACKAY, other)
4. Use QSAR System Program or Medchem
5. Use an expert guess (or terminate the session)

* May be calculated by the program with a SAR (fill in -1). Either solubility or octanol-water partition coefficient must receive a value!

✓ Value not required when program SAR’s are not used

<table>
<thead>
<tr>
<th>Parameter</th>
<th>nominal</th>
<th>worst case</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular mass (g/mol)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Saturated vapour pressure at 20 °C (Pa)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Solubility at 20 °C (g/m³)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Melting temperature (°C)</td>
<td>⋯</td>
<td>⋯</td>
</tr>
<tr>
<td>Proton dissociation constant ($^{-10}$ log mol/l)</td>
<td>⋯</td>
<td>⋯</td>
</tr>
<tr>
<td>Octanol-water partition coefficient ($^{-6}$ log l/kgOC)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Partition coefficient ($^{-6}$ log l/kgOC)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Relative partition coefficient DOC (-)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Bioconcentration factor ($^{-6}$ log kg/kg lipids)</td>
<td>⋯</td>
<td>⋯ (high)</td>
</tr>
<tr>
<td>Henry’s constant at 20 °C (Pa.m³/mol)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Degradation rate fresh water at 20 °C (1/day)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Degradation rate fresh sediment at 20 °C (1/day)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Degradation rate marine water at 20 °C (1/day)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Degradation rate marine sediment at 20 °C (1/day)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
<tr>
<td>Degradation rate atmosphere at 20 °C (cm²/molec/sec)</td>
<td>⋯</td>
<td>⋯ (low)</td>
</tr>
</tbody>
</table>
b) Supply data for ecotoxicological characteristics.

Comments:
Species group number:
1 algae, 2 bivalves, 3 amphipods, 4 echinoderms, 5 roundfish, 6 eel
Determine values using the prescribed selection procedures.

<table>
<thead>
<tr>
<th></th>
<th>water (g/m³)</th>
<th>sediment (g/kgOC)</th>
<th>biota (g/kgWW)</th>
<th>species group biota (number)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEC</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>EC50</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

The selection procedures are explained in section 3.5.2 of part I of this report.

4.3 Transport and retention

The first menu in this section presents the following list of input files concerning the physical properties and the water quality of compartments in river basins:

Water volume ($V_w$)
Flow rate ($Q_o$)
Suspended solids concentration ($S_s$)
Dissolved organic carbon concentration ($C_{doc}$)
Phytoplankton concentration ($C_{phy}$)
Transfer coefficient water film ($k_w$)
Transfer coefficient gas film ($k_g$)
Surface area ($A_w$)
Settling rate ($v_s$)
Fraction organic matter in sediment ($f_{om}$)
Fraction sand in sediment ($f_{sand}$)
Porosity ($\phi$)
Sediment volume ($V_s$)

The second screen allows editing of a selected input file.
4.4 Emission data

Four subsections are passed through according to the needs of the user. The first screen allows selection of:

- Observed loads
- Prefixed emissions
- Estimated emissions
- Boundary concentrations

Figure 4.1 gives an overview of the possibilities that the user has to compose a loading scenario for the North Sea, with respect to aquatic emissions. Imposing of atmospheric emissions proceeds in a similar way. However the atmospheric emissions are aggregated on a country level, and may either be prefixed or estimated.
4.4.1 Observed loads

The use of observations for quantification of loads is preferred to estimation of emissions, if sufficient and reliable data are available. This section is split up into two parts:

Select river basins and seasons
Provide observations

The respective second screens read:

a) Give the locations in the selected river basins for which you want to use observations and indicate the type of water system at these locations.

Comments:
No observations used: 0
Locations: river up - (1) - river down - (2) - estuary - (3) - North Sea
Type of water system: 1 = sluice, 2 = mixed river, 3 = rain river

<table>
<thead>
<tr>
<th></th>
<th>winter</th>
<th>spring</th>
<th>summer</th>
<th>autumn</th>
</tr>
</thead>
<tbody>
<tr>
<td>river A</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>river B</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>river N</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
</tbody>
</table>

Notice that for each season only one location may be provided for a river basin.

b) Provide the observations.

Comments:
You may provide data as many as you like.
Concentration C in g.m³, flow rate Q in m³.day⁻¹.
Leave fields empty when no data are available.

<table>
<thead>
<tr>
<th>River</th>
<th>winter C</th>
<th>winter Q</th>
<th>spring C</th>
<th>spring Q</th>
<th>summer C</th>
<th>summer Q</th>
<th>autumn C</th>
<th>autumn Q</th>
</tr>
</thead>
<tbody>
<tr>
<td>river A</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>river A</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>river B</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>river N</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
</tbody>
</table>
The program determines the type of substance, 1 when >50% dissolved, 2 when >50% adsorbed. Although daily flow rates will be generally available, as they must have been used to quantify season average flow rates, they may not be at hand for the user. A simple load calculation method will be applied when flow rate data are not provided. The load calculation method is determined as follows:

1) When values are not provided for the flow rate, when number \( n \) of observations < 3 or when system type 1, method 1 and accuracy intervals 2 are applied.
2) When \( n > 2 \), system type 2 and substance type 1, method 2 and accuracy intervals 2 are applied.
3) When \( n > 2 \), system type 2 and substance type 2, method 3 and accuracy interval 3a are applied.
4) When \( n > 2 \), system type 3 and substance type 1, method 2 and accuracy interval 2 are applied.
5) When \( n > 2 \), system type 3 and substance type 2, Method 3 and accuracy interval 3b are applied.

The methods are described in part 1, section 3.1.2. Loads are calculated as the 90-percentile value of the load probability distributions, which is in line with a worst case approach.

### 4.4.2 Prefixed emissions

As appears from the first screen in this section, the prefixed emissions may refer to:

- Emissions into the atmosphere
- Emissions into river basins
- Emissions into the North sea
- Background atmospheric deposition

Prefixed emissions should be provided, when reliable data are ready at hand, when more specific (better) estimation methods are available than provided by the screening program, or when a specific hypothetical case is to be considered.

The respective second screens read:

a) Provide prefixed emissions into the atmosphere (g/day).

**Comments:**

The vapour phase fraction of the emitted substance will be subject to degradation in the atmosphere. The aerosol-bound fraction is considered stable to photochemical degradation.
b) Provide prefixed emissions into river basins (g/day).

<table>
<thead>
<tr>
<th></th>
<th>winter</th>
<th>spring</th>
<th>summer</th>
<th>autumn</th>
</tr>
</thead>
<tbody>
<tr>
<td>country A</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>country B</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>country N</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>winter</th>
<th>spring</th>
<th>summer</th>
<th>autumn</th>
</tr>
</thead>
<tbody>
<tr>
<td>river A</td>
<td>drain up</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td></td>
<td>drain down</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td></td>
<td>river up</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td></td>
<td>river down</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td></td>
<td>estuary</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>....</td>
<td>drain up</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>river N</td>
<td>drain down</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td></td>
<td>river up</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td></td>
<td>river down</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td></td>
<td>estuary</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
</tbody>
</table>

c) Provide prefixed aquatic emissions for the North Sea (g/day).

<table>
<thead>
<tr>
<th></th>
<th>winter</th>
<th>spring</th>
<th>summer</th>
<th>autumn</th>
</tr>
</thead>
<tbody>
<tr>
<td>North Sea zone A</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>North Sea zone B</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
<tr>
<td>North Sea zone N</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
</tr>
</tbody>
</table>

Only the fields of selected seasons are accessible in screens a-c.

d) Provide data on the background atmospheric deposition.

**Comments:**
If the aerosol-bound fraction is >0.1 and the half life time >20 days, this substance may be transported over very long distance. Background deposition due to emissions from outside Europe could therefore occur. Deposition fluxes based on European emissions only may underestimate actual fluxes. Otherwise, background deposition due to emissions from outside Europe may be ignored.

Option 1: Provide background deposition flux (g/m²/day)
Option 2: Provide background atmospheric concentration (g/m³)

Option

Flux or concentration

....

....

de i f t hydraulics | w l
4.4.3 Estimated emissions

This section contains two subsections:

Select countries
Provide emission related data

The total emissions of the selected countries are calculated as if the countries shape up a homogeneous area. The emissions are distributed among the individual countries (atmospheric emissions) and drainage areas of river basins (aquatic emissions). Corrections are carried out if:

- an individual country has been assigned prefixed atmospheric or aquatic emissions;
  or
- an individual river basin has been assigned 'observed' aquatic loads.

The estimated values are replaced with 'observed' and 'prefixed' values. A corrective procedure is executed to prevent 'double counting' of emissions. The observed and prefixed loads are subtracted from the total estimated emission. A negative result is set to zero. A positive result is distributed among countries, riverbasins and the downstream compartments of the river basin concerned. This procedure may cause unrealistic spreading of emissions. The user may counteract this by providing more prefixed emissions.

The respective second screens read:

a) Select countries for which emissions will be estimated.

Comments:
1) If required data are available, they are usually available for the EC as a whole, whereas data on individual countries may be hard to obtain. Generally, it is recommended to consider joint emissions of EC-countries. Exceptions for specific countries or river basins, for which reliable data are available, can be made through the subsections 'observed loads' and 'prefixed emissions'. The HEDSET approach has been developed for EC-countries. Involving other countries implies extrapolation of EC-data, which may not be justified.
2) Different emission formulas are used for substances used in agriculture than for other substances.

Select: (0=no/1=yes)

1 country A
1 country B
0 ......
1 country N
Emission to water : 1

to atmosphere : 1

Indicate the type of use of the substance.
Select: (1 = agriculture, 0 = other)

....

The response of the subprogram is that selected countries are given index 'yes'. Other countries will not be considered by the emission estimation module. The user may rule out estimated emissions to either the atmosphere and/or the water compartments. He must then provide prefixed emissions or observed loads in stead.

b) Provide overall mass balance data for the selected countries and emission factors for the five life cycle stages.

Comments:
1) In case only one season is considered because emission mainly takes place in that particular season, yearly average values given in g/day are to be multiplied with 4. In other cases the average yearly values are to be used.
2) The emission factors can be quantified as functions of the main category, the industrial category, the saturated vapour pressure and the solubility. For this, tables have been provided as part of the manual.

Mass balance:

Production .... (g/day)
Import .... (g/day)
Export .... (g/day)

Emission factors atmosphere:

Production: .... (-)
Formulation: .... (-)
Processing: .... (-)
Private use .... (-)
Recovery .... (-)

Emission factors water:

Production: .... (-)
Formulation: .... (-)
Processing: .... (-)
Private use .... (-)
Recovery .... (-)
The user has to assign a main use category and an industrial use category to the substance, and look up the appropriate emission factors. The tables needed are provided in Appendix A. The HEDSET main categories are:

I Application in closed systems
II Application resulting in matrix inclusion
III Non-dispersive application
IV Wide dispersive application

The HEDSET industrial categories are:

1 Agricultural industry
2 Chemical industry, basic chemicals
3 Chemical industry, chemicals used in synthesis
4 Electrical, electronic engineering industry
5 Personal/domestic application
6 Public domain
7 Leather processing industry
8 Metal extraction, refining and processing industry
9 Mineral oil and fuel industry
10 Photographic industry
11 Polymers industry
12 Pulp, paper and board industry
13 Textile processing industry
14 Paint, lacquer and varnish industry
15 Others

The remaining factors required for geographical distribution and calculation of emissions have been provided in the program. They concern:

- the percentages of urban and agricultural landuse in EC-countries; and
- the retention factor for sewage treatment plants as a function of Henry’s constant and the octanol-water partition coefficient.

4.4.4 Boundary concentrations

The first and only screen in this section allows to adjust the concentrations at the two open boundaries of the North Sea. The screen reads:

Supply total concentrations for all open North Sea Boundaries.

<table>
<thead>
<tr>
<th></th>
<th>winter</th>
<th>spring</th>
<th>summer</th>
<th>autumn</th>
<th>scaling (x g/m³)</th>
<th>(g/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>'Atlantic'</td>
<td>1 10⁶</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>(g/m³)</td>
<td></td>
</tr>
<tr>
<td>'Channel'</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>....</td>
<td>(g/m³)</td>
<td></td>
</tr>
</tbody>
</table>

The scaling factor is fixed. Changing the value in the screen does not affect calculations.
5 Execution and output

The remaining menus under main sections 'Emission', 'River basins', 'North Sea' and 'Output' allow the user either to execute a subprogram or to view output. The following output may be viewed:

- section Emission: - a log file, giving information on computational steps
  - the calculated emissions for all compartments

- section River basins: - a log file, giving information on computational steps
  - the calculated loads for all river basin compartments,
    nominal results and worst case results

- section Nort Sea: - none

- section Output: - graphic display of exposure concentrations, the North Sea,
  nominal results and worst case results
  - the ranking of the zones according to the calculated risks,
    nominal results and worst case results
  - the 95 percentile exposure concentrations for all zones,
    nominal results and worst case results
  - the risk classification of the zones,
    nominal results and worst case results
  - the contributions of emissions to the loads on zones,
    nominal results and worst case results

When the subprogram 'River basins' has been executed, a message may appear on the screen, telling that risks are not to be expected because the loading of the North Sea is too small. The user may then terminate or continue the computations, leave the interface or redefine the input in order to make computations for another scenario.
6 Software, hardware and installation

Software

The software of SCREMOTOX was programmed for application under DOS. The user interface was programmed in REXX, the computational subprograms in FORTRAN 77 and Microsoft FORTRAN.

It will probably take an effort of moderate size to transpose the software to a WINDOWS operated environment. The software must then be made accessible as a DOS-application, preferentially incorporated in Delft Hydraulics' Case Management Tool (CMT).

Hardware

Running of the SCREMOTOX program requires a PC with a 486-processor or Pentium processor, a VGA-screen and 6 MB RAM-memory.

Installation

The installation can be done directly by copying the programs and basic input files from diskettes to the hard disk. Directories have been specified on the SCREMOTOX diskettes.
Appendix A Emission factors, retention factors and land use factors
A.1 Introduction

The tables in Appendix A provide the emission factors, that have to be specified for each of the life cycle stages in the input of SCREMOTOX. The stages are: production (1), formulation (2), processing (3), private use (4) and recovery (5). The interpretation of the main categories and the industrial categories is not always straightforward. Some important indications are given below.

A.2 The main categories (MC’s)

USES and HEDSET (Harmonized Electronic Data Set) allow for only one entry of the MC for all stages of the life cycle. However, life cycle stages may relate to different main categories. The interpretation of main categories is specified below.

<table>
<thead>
<tr>
<th>MC</th>
<th>Stage</th>
<th>Interpretation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ia</td>
<td>Production</td>
<td>Non-isolated intermediates (IC = 3, UC = 33)</td>
</tr>
<tr>
<td>Ib</td>
<td>Production</td>
<td>Isolated intermediates stored on-site, or substances (other than intermediates) produced in a continuous production process</td>
</tr>
<tr>
<td>Ic</td>
<td>Production</td>
<td>Isolated intermediates stored off-site, or substances (other than intermediates) produced in dedicated equipment</td>
</tr>
<tr>
<td>II</td>
<td>Formulation</td>
<td>Inclusion into or onto a matrix</td>
</tr>
<tr>
<td></td>
<td>Processing</td>
<td>Inclusion into or onto a matrix</td>
</tr>
<tr>
<td>III</td>
<td>Production</td>
<td>Multi-purpose equipment</td>
</tr>
<tr>
<td></td>
<td>Formulation</td>
<td>Multi-purpose equipment</td>
</tr>
<tr>
<td></td>
<td>Processing</td>
<td>Non-dispersive use (industrial point sources)</td>
</tr>
<tr>
<td>IV</td>
<td>Processing</td>
<td>Wide dispersive use (many small point sources or diffuse releases; normally no emission reduction measures)</td>
</tr>
</tbody>
</table>

A.3 The industrial categories (IC’s)

The industrial categories specify the branch of industry (including personal and domestic use, and use in the public domain), where considerable emissions occur at application of the substance as such, or at the application and use of preparations and products containing the substance. Some important emission sources have not been included specifically in this scheme and hence have to be allocated to category "Others" (no. 15/0), e.g. emissions of substances (in preparations) other than fuels and fuel additives used in motor vehicles.
It should be noted that considerable emissions may occur at another category than the one where a substance has been allocated to. A substance used in a paint will be allocated to IC 14 "Paints, lacquers and varnishes". Though the local emissions of solvents may be considerable at one point source (the paint factory) at the stage of formulation (paint production), most of the solvent will be emitted at paint application. The application could be classified in several industrial categories depending on the type of paint. In case of a do-it-yourself paint it would belong to IC 5 "Personal/domestic", in case of motor car repair or professional house painting it would be IC 15/0 "Others" (wide dispersive use) and in case of motor car production 16 "Engineering industry: civil and mechanical" (non-dispersive use, implying a few large point sources).

It is possible that confusion arises when the use of a substance, belonging to a certain specific process of an industrial category, occurs at another branch of industry. An example is the application of an additive for an epoxy resin applied in the electronic industry for the embedding of electronic components. Though the processing takes place at IC 4 "Electrical/electronic engineering industry" the processing of epoxy resins belongs to IC 11 "Polymers industry". The releases of the process will be found in the table for the latter category.

For chemical industry, two separate industrial categories exist, one for basic chemicals and one for chemicals used in synthesis. Basic chemicals are considered to comprise commonly used chemicals such as solvents and pH-regulating agents such as acids and alkalis. Also the primary chemicals from the oil refining process are considered as basic chemicals. Chemicals used in synthesis fall in two classes, namely intermediates (substances produced from a starting material to be converted in a subsequent reaction into a new substance) and other substances. These other substances consist mainly of "process regulators" (e.g. accelerators, inhibitors, indicators). For industrial category 5 (personal/domestic) the use and application of substances (as such or in formulations) is considered at the scale of households. The types of application are adhesives, cosmetics, detergents and pharmaceuticals. Some applications have been covered in other industrial categories at the stage of private use. These applications comprise fuels and fuel additives (mineral oil and fuel industry) and paint products (paints, lacquers).
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<th>Disp.f.</th>
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**Waste water**

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Soil
### Table A3.1 Release estimates for industrial category 1 (Agricultural industry) at processing

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### Soil

---

delft hydraulics | W1
### Table A3.4 Release estimates for industrial category 4 (Electrical/electronic engineering industry) at processing

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### Table A3.5 Release estimates for industrial category 6 (Public domain) at processing

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### Table A3.6 Release estimates for industrial category 7 (Leather processing industry) at processing

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### Table A3.8 Release estimates for industrial category 9 (Mineral oil and fuel industry) at processing

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### Table A3.9 Release estimates for industrial category 10 (Photographic industry) at processing

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*solid materials (e.g. films)/Main category II*

| Waste water | 0.8 | 1.2 |
| Soil        |     |     |

### Table A3.10 Release estimates for industrial category 11 (Polymers industry) at processing

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<td>0.025</td>
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<p>| Waste water | 0.0005 | 3    |
| Soil        |        |      |</p>
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Table A3.12  Release estimates for industrial category 13 (Textile processing industry) at processing

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<th>Release</th>
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Soil
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<td>0.225</td>
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<td></td>
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<td>0.075</td>
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### Table A4.2 Release estimates for industrial category 9 (Mineral oil and fuel industry) at private use

<table>
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<th>Conditions</th>
<th>Release</th>
<th>Disp.f.</th>
</tr>
</thead>
<tbody>
<tr>
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<td>vapour pr.(Pa)</td>
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<td></td>
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<tr>
<td></td>
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<td>0.0001</td>
<td>5</td>
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<td></td>
<td></td>
<td>1 - 10</td>
<td>0.005</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>10 - 100</td>
<td>0.01</td>
<td>2</td>
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<tr>
<td></td>
<td></td>
<td>100 - 1,000</td>
<td>0.025</td>
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<td></td>
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<td>0.05</td>
<td>2</td>
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<td>Waste water</td>
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<td></td>
<td>0.0005</td>
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</table>

Soil

---

delft hydraulics | WL
### Table A4.3 Release estimates for industrial category 10 (Photographic industry) at private use

<table>
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<tr>
<th>Compartment</th>
<th>Remarks</th>
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<th>Release</th>
<th>Disp.f.</th>
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<td>Soil</td>
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### Table A4.4 Release estimates for industrial category 13 (Textile processing industry) at private use

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<th>Release</th>
<th>Disp.f.</th>
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</thead>
<tbody>
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<td></td>
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<td>Waste water</td>
<td>solubility (mg/l)</td>
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<td>250 - 1,000</td>
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<td>1,000 - 5,000</td>
<td>0.2</td>
<td>1.5</td>
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<tr>
<td></td>
<td></td>
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<td>0.3</td>
<td>1.2</td>
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<td>Soil</td>
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### Table A4.5 Release estimates for industrial category 14 (Paints, lacquers and varnishes industry) at private use

<table>
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<th>Conditions</th>
<th>Release</th>
<th>Disp.f.</th>
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<tr>
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<td>1 - 10</td>
<td>0.01</td>
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<td></td>
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<td>10 - 100</td>
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<td>Soil</td>
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### Table A4.6 Release estimates for industrial category 15 (others) at private use

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<tbody>
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<td>vapour pr.(Pa)</td>
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<td></td>
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<td></td>
<td>&lt;10</td>
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<td>solubility (mg/l)</td>
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<td>0.01</td>
<td>5</td>
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<tr>
<td></td>
<td></td>
<td>10 - 100</td>
<td>0.1</td>
<td>2.5</td>
</tr>
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<td></td>
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<td>0.4</td>
<td>1.5</td>
</tr>
<tr>
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<td></td>
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<td>0.8</td>
<td>1.2</td>
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### Table A5.1 Release estimates for industrial category 10 (Photographic industry) at recovery

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<th>Conditions</th>
<th>Release (Pa)</th>
<th>Disp.f.</th>
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<td>$5 \times 10^{-6}$</td>
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<td></td>
<td></td>
<td>1 - 10</td>
<td>$2.5 \times 10^{-6}$</td>
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<tr>
<td></td>
<td></td>
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<td>0.00075</td>
<td>10</td>
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<tr>
<td></td>
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<td>100 - 1,000</td>
<td>0.0025</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\geq 1,000$</td>
<td>0.01</td>
<td>6</td>
</tr>
<tr>
<td>Waste water</td>
<td></td>
<td></td>
<td>0.2</td>
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</tr>
<tr>
<td>Soil</td>
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### Table A5.2 Release estimates for industrial category 12 (Pulp, paper and board industry) at recovery

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<th>Release</th>
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<tbody>
<tr>
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</tr>
<tr>
<td>Waste water</td>
<td></td>
<td></td>
<td>0.2</td>
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</tr>
<tr>
<td>Soil</td>
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### Table A5.3 Release estimates for industrial category 15 (Others) at recovery (if applicable)

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<tbody>
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</tr>
<tr>
<td>Soil</td>
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Retention factors for sewage treatment plants

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<table>
<thead>
<tr>
<th>Kow</th>
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<tbody>
<tr>
<td>&lt; 10</td>
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<td>-----</td>
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<tr>
<td>H</td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td>&lt; 2</td>
</tr>
<tr>
<td>2 - 3</td>
</tr>
<tr>
<td>3 - 4</td>
</tr>
<tr>
<td>4 - 5</td>
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<td>5 - 6</td>
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Calculated from Struis et al., 1991.

Land use factors

Factors directly relate location with the EC

Water emissions

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<th>fac_agricult</th>
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<tr>
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<tr>
<td>river_upstream</td>
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</tr>
</tbody>
</table>
addresses

delft hydraulics

Decisive advice: from multidisciplinary policy studies to design and technical assistance on all water-related issues.

location Delft
Rotterdamseweg 185
p.o. box 177
2600 MH Delft
The Netherlands
telephone +31 15 2569353
telefax +31 15 2619674
telex 38176 hydel-nl
e-mail info@wldelft.nl

location 'De Voorst'
Voorsterweg 28, Marknesse
p.o. box 152
8300 AD Emmeloord
The Netherlands
telephone +31 527 242922
telefax +31 527 243573
telex 42290 hydvo-nl
e-mail info@wldelft.nl