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REIMSEA: an LCA toxicity characterization model for the North Sea

Wegener Sleeswijk, A.; Kleijn, R.; Karman, C.; Bernhard, R.; Vlies, L. van der

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REIMSEA: AN LCA TOXICITY CHARACERIZATION MODEL FOR THE NORTH SEA

REIMSEA: AN LCA TOXICITY CHARACTERIZATION MODEL FOR THE NORTH SEA

Supplement to 'REIM: LCA-based Ranking of Environmental Investment Model' including toxicity characterization factors for 12 organics and 7 metals

Anneke Wegener Sleeswijk
René Kleijn
Chris Karman
Roland Bernhard
Liesbeth van der Vlies

Centrum voor Milieukunde
Universiteit Leiden
Postbus 9518
2300 RA Leiden

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PREFACE

This study was performed by CML (Centre of Environmental Science, Leiden University) in co-operation with TNO-MEP (TNO Environment, Energy and Process Innovation) and was commissioned by NOGEPA ('Netherlands Oil and Gas Exploration and Production Association'), of which NAM is a member.. The report consists of two parts. Part I is a description of the actual model, including all collected data and modelling results. In the REIMSEA model, specific attention has been paid to the behaviour of metals in sea water compartments. Part II is a general treatise on immobilisation of metals in North Sea and ocean. TNO-MEP was mainly responsible for Chapter 4: *Substance Choice and Data*, for the appendices B and C – the parts of the study concerned with the collection of physicochemical data, toxicity data and data on degradation rates – and for part II.

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1 INTRODUCTION

1.1 The use of LCA

Environmental assessment of process alternatives or improvement options in the offshore industry can be tested on different levels. Changes in location-specific risk levels can be analysed with risk models such as CHARM III (Karman *et al.*, 1996) or SCREMOTOX (WL/Delft Hydrolics *et al.*, 1996). For the more general investigations of improvement options, that usually precede these more specific studies, life cycle assessment (LCA) is in several respects a more appropriate tool:

- LCA encompasses the entire life cycle;
- LCA encompasses a broad scope of environmental impacts;
- LCA includes quantitative impact scores on a limited number of environmental impact categories;
- LCA offers the possibility to compare improvement options on a functional basis.
- LCA is location-independent;

Below, each of these points will be elaborated.

Encompassing both the entire life cycle and a broad scope of environmental impacts is necessary to ensure that 'problem shifting' will be avoided. Problem shifting occurs when environmental improvements in a certain region and/or with respect to a certain impact category are coupled to reinforcement of environmental problems in other regions or with respect to other impact categories. Impact categories include not only ecotoxicity and human toxicity, but also reinforcement of the greenhouse effect, depletion of the ozone layer, acidification, eutrophication, photochemical oxidant formation and resource depletion.

Quantitative impact scores on a limited number of environmental impact categories make it possible to get an easily surveyable image of the overall environmental effects of the options to be assessed, so that quantitative comparisons can be made for each impact category.

The possibility to compare improvement options on a functional basis means that differences in production efficiency, life time of a product, recycling rate etc., which make product alternatives difficult to compare as such, are taken into account in a quantitative procedure.

Location independence makes it possible to compare process alternatives as such, independent of the exact location where the process will take place. Such comparisons are necessary as a support for decisions on general process changes that are not location-bound.

1.2 LCA: some recent developments

Some recent developments in LCA-methodology include incorporation of fate information and the use of a region-specific approach in life cycle impact assessment.

Environmental fate of chemicals encompasses both intercompartmental transport and environmental degradation and immobilisation. Intercompartmental transport refers to both intermedia transport and transport between regionally differentiated compartments within one medium (e.g. 'North Sea air' versus 'Dutch air'). Degradation rates may differ between compartments. 'Mackay-type' multimedia fate models can conveniently be used for LCA-fate modelling. In these models, compartments are assumed to be homogeneously mixed. Diffusive and advective transport rates between and degradation rates within compartments are described by

mathematical equations. Multimedia fate models are now being used for LCA toxicity assessment in LCA. Huijbregts *et al.* (2000) has developed LCA toxicity characterization factors, based on the fate and exposure model USES 2.0, that have been included in the CML LCA Guide (Guinée, 2002).

Another recent development in life cycle impact assessment is regional differentiation (*cf.* Potting, 2000). Region-specific information in the context of life cycle impact assessment can be distinguished in three categories:

- information on environmental properties;
- exposure-related information;
- effect-related information.

Information on environmental properties refers to climatological properties (temperature, wind speed, rain rate) and geographical and geological information (water coverage, soil type). These parameters are determinant for the distribution of chemicals between environmental compartments as well as degradation rates within these compartments, or, in other words, for environmental substance fate.

Exposure related information largely refers to human food consumption patterns and the relationship between environmental concentrations and different human exposure routes. Biological availability in included in the effect parameters.

Effect related information refers to parameters that determine the sensitivity of a region to certain emissions: background concentrations, biological availability, the presence of sensitive species and species abundance or (human) population density.

1.3 The use of LCA in the offshore-industry

In the offshore-industry, LCA is being used to calculate the cost-effectiveness of environmental measures. In order to make it possible to use LCA for this specific purpose, NAM ('Nederlandse Aardolie Maatschappij BV') commissioned CML in 1993 to develop a supplementary module to the existing CML LCA-model (Heijungs *et al.*, 1992). This supplementary model was named REIM (Wit *et al.*, 1993).

The REIMSEA model presented in this report was commissioned by NOGEPA, of which NAM is a member. The most important goal of the REIMSEA project was to expand the REIM model with region specific LCA toxicity characterization factors for the North Sea – the most relevant emission region for NOGEPA. A second goal was to adapt the fate model underlying these characterization factors with respect to metals, especially regarding metal behaviour in the marine environment.

The ECB model EUSES 1.00 (ECB, 1997) was used as a modelling basis. A North Sea module was added to a reprogrammed version of the EUSES 1.00 model, and some further model-adaptations were made to adapt the model with respect to the goals of this project. Toxic effect-assessment for ecotoxicity was updated as well. In the next chapter, all adaptations and additions are described in detail. In appendix A, characterization factors, calculated with this additional module, are given for a set of 19 chemicals, selected by NOGEPA and TNO-MEP. All these substances are emitted in substantial amounts by the offshore industry. This update has been limited to wo effect types: human toxicity and ecotoxicity.

2 A NORTH SEA FATE AND EXPOSURE MODEL FOR LCA

2.1 Specific adaptations of the EUSES 1.00 model

In the North Sea offshore-industry, the introduction of process alternatives may be considered for large parts of the region, or even for the entire North Sea. Environmental comparisons of such process alternatives should be location-independent on the one hand, while on the other hand, they should preferably be tailored to the specific region to which the assessment refers. The North Sea region as a whole seemed to be the most appropriate level of assessment.

In the EUSES 1.00 model, three levels of distribution areas are distinguished: a local, a regional and a continental level. The local scale is accounted for by a separate dispersion model, which has not been implemented in the context of the REIMSEA model. The regional level concernes larger regions (such as separate countries), and the continental level is defined as the sum of all EU member states. In the framework of the REIMSEA project, both the regional and the continental level were represented by two separate areas: the regional level by both The North Sea and The Netherlands, and the continental level by both the total ice-free areas of world oceans and world continents, respectively. The total area is handled as a closed environmental system. Contrary to the EUSES 1.00 model, the REIMSEA model does not only consider trans-boundary transport from the regional to the continental level, but also vice versa. Although the model scale is expanded from the the EU to the global scale, the environmental parameters for the continental system were left unchanged.

On the basis of a consensus in the steering group of the REIMSEA project, the environmental effects of substances which reach the oceans can be considered to be negligible for some applications. This is especially important for metals, since these non-degradable substances spend most of their environmental lifetime in the oceanic waters, before eventually settling down in the sediment The point of view that it should be possible to leave metals in the ocean out of consideration was taken into account by calculating two sets of characterization factors: one for the system as a whole (conform common LCA practice), and one that leaves out exposure to substances in the oceanic area.

In a model-technical sense, the REIMSEA model can be considered as a precursor of the GLOBOX model that is currently developed at CML: a global, regionalized multimedia fate and exposure model for LCA that considers trans-boundary exchange of substances between all the different countries of the world, and the world oceans. The distinction of the North Sea as a separate region with separate characterization factors is, however, specific for the REIMSEA model.

2.2 Adaptations with respect to LCA

Multimedia models such as EUSES 1.00 have not been specifically developed for LCA-purposes. This implies that they may have qualities that are undesirable for LCA-applications. A drawback of the use of EUSES 1.00 for LCA-applications is the fact that the environmental system is not closed: substance flows leaving the area of the EU are not involved in the calculations. For LCA, it is important that substances are included in the assessment as long as they exist in the environment as a whole, not just a region.

In the RIVM model SimpleBox 2.0 (Brandes *et al.*, 1996), which forms the basis of the fate module in EUSES 1.00 model, the environmental system encompasses not just the EU, but the entire

northern hemisphere. A closed system is created here by extending the environmental system to a global level with three global scales (tropic, moderate, and arctic), representing the northern hemisphere, with mutual flows between the air and sea compartments between the moderate scale on the one hand and the tropic and arctic scale on the other hand (Brandes *et al.*, 1996). For the REIMSEA model, a simpler solution is used: the North Sea, the world ocean ('atlantic' in the model), The Netherlands ('regional' in the model) and the global land area ('continental' in the model). These are considered to form the closed 'unit world'. Contrary to EUSES 1.00, the REIMSEA model is constructed in such a way that trans-boundary transport exists not only from the regional to the continental system, but also in the opposite direction.

2.3 Environmental parameters of the regions 'North Sea' and 'ocean'

The original EUSES 1.00 model contains six environmental compartments for both the regional and the continental system: air, water, sediment, natural soil, agricultural soil and industrial soil. In the REIMSEA model, suspended matter and biota are considered as separate compartments, rather than as parts of the bulk compartment 'water'. This approach (which has been implemented accoriding to the original SimpleBox 1.0 model (Van de Meent, 1993, has also been folowed for the sea systems. Five compartments were added to the for each of the regions 'North Sea' and 'ocean': sea air, seawater, sea suspended matter, sea biota and sea sediment. The North Sea adapted model thus contains 26 environmental compartments.

2.4 Adaptations with respect to processes within sea- and ocean compartments

The inflows to the North Sea water and suspended matter compartments were assumed to result from 10 European rivers and from three seawater inflows. All these inflows were summarised to four main flows: riverine and oceanic inflows of water and suspended matter, respectively. It should be observed that this implies that the Baltic Sea is handled as part of the ocean compartment in this model. The riverine and oceanic water inflows to the North Sea were assumed to be exactly counterbalanced by a water outflow into the oceans, corresponding to a refreshment time of 1 year for the North Sea as a whole. Riverine inflows to the oceans were also considered, on a global scale. The suspended matter, contained in the riverine inflows to North Sea and oceans, was assumed to sediment for 90 percent to the sea floor on the river-sea boundary (Chester, 1990). The surplus on the water balance, caused by the fact that inflows to the oceans are not counterbalanced by any outflows, was assumed to evaporate. The hydrological cycle is closed by the precipitation of evaporated water as rain and snow, that bring back water to the continents. When water evaporates from the ocean compartment, dissolved contaminants are left behind. Since these contaminants will eventually leave the environmental system by sedimentation, this does not disturb the steady-state based multimedia equations.

Exchange between the different air compartments has also been considered. Half of the airflow, leaving the Netherlands, was assumed to go to the world continents; the other half was assumed to go to the North Sea. 20 percent of the airflow that leave the North Sea system was assumed to go to the world oceans; the remaining airflows were assumed to go to the Netherlands and the continental system.

Since the air compartment in EUSES 1.00 consists of only one layer, a common wind speed had to be chosen for the entire system. Since the North Sea area plays the central role in this model, a North Sea specific values was chosen for this parameters: 5.8 meter per second (ICONA, 1992, and Smits *et al.*, 1996, average value).

Advective transport from air to other media is influenced by the fraction of the airborne concentration that is associated with aerosols. This fraction depends, among others, on the particle concentration in the air, or, more precise, on their collective surface area. In the EUSES 1.00 model, the product of the so-called 'constant of Junge' and the surface area of aerosols is set to a fixed value. Since the concentration of aerosols in sea air is considerably lower than in air in land-covered areas, this value was considered to be inappropriate for sea-covered areas. It was therefore detached from the constant of Junge (which was assumed to be 0.17 Pa×m; Noordijk & De Leeuw, 1991), and set to a separate value for the North Sea and ocean air compartments.

The North Sea water and suspended matter compartments were assumed to be completely mixed over the full North Sea depth. The equivalent ocean compartments were, however, considered to consist of different mixing layers. Only the upper mixed layer was considered as part of the environment to be assessed. The depth of this layer was assumed to be a 100 metres; slightly more than the assumed average North Sea depth of 90 metres. Up- and downwelling were not considered; only settling suspended matter was assumed to cross the boundary between the upper ocean water layer and the water layer below.

In EUSES 1.00, net sedimentation is defined as the difference between ingoing and outgoing flows of suspended matter, while gross sedimentation is the sum of net sedimentation and resuspension. With the North Sea parameters collected here, this would result in a zero net sedimentation. In this model, the EUSES 1.00 equations were replaced by specific equations for the North Sea: the net sedimentation rate was derived directly form deposition velocity, and the resuspension rate from the erosion of both seafloor and coast. The gross sedimentation rate was calculated as the sum of the net sedimentation rate and the resuspension rate.

For the ocean system, the gross sedimentation rate was calculated from the average concentration of suspended matter in oceanic waters and a settling velocity, specifically calculated for oceanic waters.. Resuspension of ocean sediment was assumed to have negligible influence on concentrations in the upper layer, and was therefore set to zero. Net sedimentation was therefore considered to equal gross sedimentation. For metals, specific values for each individual metal were used for sedimentation calculations.

Degradation rates in saline surroundings were assumed to be factor 0.7 below the equivalent degradation rates in freshwater environments. Sea water and sea sediment half-life times were therefore derived from freshwater values by division by 0.7 (Karman *et al.*, 1998).

The environmental parameters used to describe the REIMSEA environmental systems are listed in the tables 2.4.1 – 2.4.6 (as far as they differ from the parameters, used in the EUSES 1.00 model).

Table 2.4.1 Specific REIMSEA parameters of all systems

parameter [unit]	symbol	value
average wind speed [$m \cdot s^{-1}$]	WINDSPEED	5.8[a]

[a] North Sea Task Force (1993); ICONA (1992); RWS DGW/RIZA/Noordzee (1993) (average value)

Table 2.4.2 Specific REIMSEA parameters of the regional system

parameter [unit]	symbol	value
sum of riverine inflows [$m^3 \cdot s^{-1}$]	INFLOW_water	2600[a]
human population [inhabitants]	POPUL	1.5×10^{7} [a]

[a] World Resources Institute (2002)

Table 2.4.3 Specific REIMSEA parameters of the continental system

parameter [unit]	symbol	value
total area [m^2]	SYSTEMAREA	1.5×10^{14} [a]
human population [inhabitants]	POPUL	6×10^{9} [b]

[a] Harte (1988)
[b] World Resources Institute (2002)

Table 2.4.4 Parameters of both sea systems

parameter [unit]	symbol	value
density of sea water[$kg \cdot m^{-3}$]	RHOseawater	1025[a]
average mixing depth of sediment compartment [m]	DEPTH_seased	0.1 [b]
average rain rate [$m \cdot s^{-1}$]	RAINRATE	1.9×10^{-8} [c]
average surface area of aerosol particles in air [$m^2 \cdot m^{-3}$]	SURFaer	1.5×10^{-4} [d]
temperature at the air-water interface [K]	TEMP	282 [b]

a White (2002)
[b] Karman (1998)
[c] North Sea Task Force (1993); ICONA (1992); RWS DGW/RIZA/Noordzee (1993) (average value)
[d] Smits *et al.* (1996)

Table 2.4.5 Parameters of the North Sea environmental system

parameter [unit]	symbol	value
total area [m^2]	SYSTEMAREA	0.55×10^{12} [a]
average total depth [m]	-	90 [b]
average mixing depth [m]	DEPTH_seawater	90 [b]
average concentration of suspended matter [$kg \cdot m^3$]	SUSPCONC_seawater	0.003 [b]
average production rate of suspended matter [$kg \cdot s^{-1}$]	PROD_seasusp	8.7×10^3 [c]
deposition velocity of suspended particles [kg susp$\cdot s^{-1}$]	DEPOSITION	1400[d]
sum of riverine inflows from The Netherlands [$m^3 \cdot s^{-1}$]	INFLOW_water	3113 [e]
average concentration of suspended matter in riverine inflows from The Netherlands [$kg \cdot m^{-3}$]	SUSPCONC_water	0.029 [e]
sum of riverine inflows (excluding those from The Netherlands) [$m^3 \cdot s^{-1}$]	INFLOW_water	1876 [e]
sum of seawater inflows from the oceans [$m^3 \cdot s^{-1}$]	INFLOW_seawater	1.84×10^6
average concentration of suspended matter in riverine inflows (excluding inflows from The Netherlands) [$kg \cdot m^{-3}$]	SUSPCONC_water	0.056 [e]
sum of oceanic inflows [$m^3 \cdot s^{-1}$]	INFLOW_seawater	1.84×10^6 [f]
average erosion of seafloor and coast[$kg \cdot s^{-1}$]	EROSION_seased	420 [g]
average total inflow of suspended matter from the oceans [$m^3 \cdot s^{-1}$]	INFLOW_seasusp	1.4[h]

[a] ICONA (1992); PARCOM-ATMOS (1993) (average value)
[b] Saft (1998)
[c] Karman (1998)
[d] See part II of this report, page 15 (mass balance)
[e] ICONA (1992); RWS DGW/RIZA/Noordzee (1993); anonymous (1996)
[f] Villars (1998); RWS DGW/RIZA/Noordzee (1998); Wania *et al.* (1998)
[g] See part II of this report, page 15 (mass balance)
[h] Calculated from data in part II of this report, page 15(mass balance)

Table 2.4.6 Parameters of the ocean environmental system

parameter [unit]	symbol	Value
total area [m^2]	SYSTEMAREA	3.28×10^{14} [a]
average mixing depth [m]	DEPTH_seawater	100 [b]
sum of riverine inflows [$m^3 \cdot s^{-1}$]	INFLOW_water	1.3×10^{6} [c]
average concentration of suspended matter [$kg \cdot m^3$]	SUSPCONC_seawater	0.00009 [d]
average production rate of suspended matter [$kg \cdot s^{-1}$]	PROD_seasusp	6.3×10^{4} [e]
average total inflow of suspended matter from the North Sea [$m^3 \cdot s^{-1}$]	INFLOW_seasusp	4.7 [f]
settling velocity of suspended matter [$m \cdot s^{-1}$]	SETTLvelocity_seasusp	1.85×10^{-6} [g]

[a] Harte (1988)
[b] Chester (1990)
[c] Martin & Whitfield (1983)
[d] Verbruggen *et al.*, 1997
[e] Calculated from Schulz & Zabel (2000)
[f] See part II of this report, page 15 (mass balance)
[g] Calculated from Salomons & Förstner (1984)

2.5 Adaptations with respect to human intake

EUSES 1.00 is a model that calculates steady state concentrations from continuous emissions. Via an intake model, these steady state concentrations can be translated to predicted daily intakes of an average member of the population, which can, in turn, be compared to a threshold value to determine the prevailing 'margin of safety' for the average population of the region under study. The emissions that are assessed with LCA are not continuous in character, since they are coupled to a *'functional unit' of product, not to the continuous production of products.* Calculations in LCA are not about steady state concentrations, but about eventual amounts of a chemical that end up in each environmental compartment, combined with the time that it will remain there before it has emerged by breakdown, immobilisation or transport to another compartment. This implies that intake calculations in LCA differ in character from the equivalent calculations in EUSES 1.00. Instead of steady-state concentrations, time-integrated amounts are calculated. It is not possible to calculate margins of safety, yet, an equivalent procedure can be followed. Reverse threshold values, such as acceptable daily intake values (ADI's) or reference doses (RfD's) are convenient weighting factors to weight the amounts of different substances that become available for human intake, due to the production of a functional unit of product. They should be supplemented, however, with a second weighting factor: the number of people exposed to the amount in each of the regions considered in the multimedia model.

For the intake of contaminants via drinking water, EUSES 1.00 uses a worst case approach: possible intakes are calculated for both groundwater and surface water based drinking water, and the highest of these two values is used in further calculations. This procedure has been replaced by a ratio 4:6 between groundwater and surface water as drinking water source which is based on the actual situation in the Netherlands (Wegener Sleeswijk *et al.*, 1996).

In the EUSES 1.00 model, human fish consumption encompasses both freshwater and seawater

fish. Although fish consumption in The Netherlands is on average largely dominated by seawater fish, it seemed appropriate to make a distinction for this sea-specific model, since fish consumption is the most direct exposure route for man to seawater emissions. For the Netherlands, the consumption of seafood and freshwater fish species could be derived from specific data on food consumption of different foodstuffs (Kistemaker *et al.*, 1993). 'Seafood' encompasses both fish and shellfish. For the rest of the world, the relative freshwater fish consumption figure was based on a rough estimate. The world total fish consumption per capita was based on the EUSES 1.00 value for the EU. Apart from seafood and freshwater fish consumptions as such, a distinction also had to be made between consumption of North Sea fish and consumption of oceanic fish, since only the consumption of North Sea fish was taken into account in this study. Seafood consumption in The Netherlands was assumed to exist for 80 percent of North Sea food, and for the remaining 20 percent of oceanic seafood. The consumption of North Sea food in the rest of the world was derived from the yearly total North Sea seafood catch by subtracting the yearly Dutch seafood consumption from the edible fraction (assumed 0.5) of this catch figure. Surplus seafood consumption of the world population was assumed to be of oceanic origin. The parameters used are listed in table 2.5.1.

Table 2.5.1 Human fish intake from different water compartments

parameter	Symbol	Value
daily intake of fresh fish by Dutch people [kg wet fish·day]	IH_fishfresh	0.0005
daily intake of North Sea fish by Dutch people [kg wet fish·day]	IH_fishnsea	0.0072
daily intake of fresh fish by world citizens[a] [kg wet fish·day]	IHcon_fishfresh	0.0010
daily intake of North Sea fish by world citizens [kg wet fish·day]	IHcon_fishnsea	0.000047

2.6 Updates, according to SimpleBox 2.0

One aspect of the RIVM model SimpleBox 2.0 (Brandes *et al.*, 1996) that has not been included in the EUSES 1.00 model is the temperature dependence of vapour pressure and degradation rates, by ways of the Clausius-Clapeyron equation. Since it seemed relevant enough, this aspect was introduced separately in the REIMSEA model.

2.7 Other adaptations

No direct emissions can take place to the 'natural soil' compartments in the original EUSES 1.00 model. This was changed in the REIMSEA model.

The REIMSEA model also attributes the possibility of direct emissions to the diverse suspended matter compartments: emissions of sludges to water bodies should be considered as emissions to the suspended matter compartment.

3 THE FATE OF METALS IN SEAS AND OCEANS

3.1 Handling metals with multimedia models

Multimedia models have been developed primarily for organic chemicals. This does not imply that these models cannot be applied at all for metals. Some adaptations are needed, however. In the first place, the estimation routines in the EUSES 1.00 model that are based on values for octanol-water partition coefficients (K_{ow}) and vapour pressures, are not fit for metals. This implies that empirical values should be gathered for a number of parameters that are usually based on estimates for organic chemicals. In the second place, the existing multimedia models do not contain routines for handling metal specific processes in fresh and marine waters and soil. And in the third place, the process of sedimentation plays such a critical role in the eventual fate of metals – especially with respect to the overall environmental residence time – that the existing modelling routines for these processes are insufficient, and should be revised on the basis of specific empirical information as far as possible.

3.2 Supplementing parameters

In table 3.2.1, the parameters for which values were not available for metals are listed, along with the (default) values that have been assigned to them. Degradation rate constants were all set to zero. For mercury, a separate set of constants is used. (See section 3.4.)

Table 3.2.1 Estimated parameter values, assigned to metal ions (except mercury)

parameter	Value	Source
air-water partition coefficient [–]	0	Mackay *et al.* (1996)
Henry's law coefficient [Pa·m^3·mole]	0	derived from air-water partition coefficient
scavenging ratio [–]	1×10^5	Crommentuijn *et al.* (1996)
fraction of chemical in air, associated to aerosol particles ($Fass_{aer}$) [–]		Crommentuijn *et al.* (1996)
zinc	0.99	
other metals	0.95	

* Due to lack of data, $K_{gas\text{-}plant}$ was set to the same value as $K_{aerosol\text{-}plant}$.

Due to lack of data, the air-plant partitioning coefficients for metals were set equal to the (general) aerosol-plant partitioning coefficient.

For human exposure modelling, a drinking water purification model, designed for organics, is used in the EUSES 1.00 model. A distinction is made between substances with a high and substances with a low octanol -water partition coefficient. Since it was expected that emissions of metals to seawater will not significantly influence drinking water, this model has not been specifically adapted for metals. If metal partitioning to freshwater and groundwater compartments occurs, metals are handled as substances with a high Kow value.

3.3 Activity

The behaviour of metals in ionic solutions, such as seawater, differs from their behaviour in fresh

water. These non-ideal effects can be taken into account by substituting concentrations by so-called 'activities' in equations describing concentration-driven environmental processes. Activities of individual substances are calculated by multiplying concentrations with activity coefficients, which depend on the ionic strength of the solute and on the electrovalence of the substance at stake. The ionic strength of seawater was assumed to be 0.7, and activity coefficients are calculated with the so-called Davies equation in the REIMSEA model. The electrovalence values, assigned to the metal ions considered for assessment in this report are presented in table 3.3.1.

Table 3.3.1 Electrovalence values, assigned to the metal ions considered for assessment

ion	electrovalence
Cadmium	2+
Chromium	3+
Copper	2+
Lead	2+
Mercury	2+
Nickel	2+
Zinc	2+

Non-ideal effects can influence the bio-availability of metal ions for uptake by water organisms, which would – at least theoretically – lower the relative toxicity of ionic substances in relation to non-ionic substances, and compared to the toxicity of equal concentrations in fresh water where these non-ideal effects are absent. The same applies for bioconcentration (factors). If test species are marine organisms, however, this effect is already accounted for by the fact that the test-medium for these organism will be saline itself. For the calculation of the characterization factors, mentioned in this report, the activity coefficients were therefore not used. If only freshwater toxicity or bioconcentration data are available, however, the user can optionally derive artificial toxicity data or bioconcentration factors for marine organisms by multiplying the toxicity value (e.g. EC_{50} or NOEC) or bioconcentration factor (BCF) by the activity coefficient provided by the REIMSEA model. It should be remarked, however, that in practice, no significant differences between freshwater and marine toxicity data could be found for at least a number of metals (*cf.* Crommentuijn *et al.*, 1997).

3.4 Speciation

One of the most well-known metal specific processes is speciation: metals tend to occur in the environment as different species. Ratios between the different species depend on regional environmental properties such as temperature and acidity, and on the medium considered. Mainly due to the presence of complexing agents in marine waters, speciation tends to differ largely between fresh and marine waters. Since most complexing agents are not present in most artificial test media, this factor is not taken accounted for by most marine toxicity data. In order to get a good picture of the relative toxicity of metals in marine surface waters, it should be accounted for separately.

Different metal species differ with respect to their chemical and toxic properties, and should actually be considered as different substances. The bio-availability of metals is believed to be largely determined by the free ion activity, rather than by the total aqueous concentration of a metal (Morel, 1983).

In the REIMSEA model, only the fraction of free ions is considered to be potentially toxic, except for mercury, for which the (highly bio-available) organic species are taken into account separately. Relative concentrations of free ions in seawater can be derived from Byrne *et al.*(1988). These values refer the ocean as a whole. Specific values for the relative amount of free ions in the mixing layer of the ocean could only be found for cadmium and zinc (Nolting *et al.*, 1999). All values are given in table 3.4.1. From the case of zinc we see that the difference between relative free ion concentrations in the ocean as a whole on the one side and in the surface layer on the other side can be enormous. For other metals than cadmium and zinc, however, we had no other choice but to apply the overall values to the surface layer as well. In the test medium, we assumed the relative free ion concentrations to equal the values reported by McGloskey (1996). For the calculation of the relative bio-availability of metal ions in sea water, we used the quotient of the relative concentration sea water (surface layer if available) and test medium, respectively.

Table 3.4.1 Relative concentrations of free ions in sea water (derived from Byrne *et al.* at T = 5°C and pH = 8.2) in the surface layer of the ocean (Nolting *et al.*, 1999), and as assumed in the test medium (McGloskey, 1996)

metal	% free ions in sea water	% free ions in surface layer	% free ions in test medium
Cadmium	3.2	0.8	71
Chromium	0.0011		91
Copper	12		76
Lead	5		40
Nickel	68		77
Zinc	73	0.9	80

3.5 Mercury speciation

Mercury takes a special place among metals, firstly because of the volatile character of its elemental species, and secondly because of the environmentally important role organometalic forms (largely methylmercury). Mackay *et al.* (1995) have introduced a 'three species model' for mercury, in which they make a distinction between elemental, inorganic, and organic mercury. For each of these groups of species, they present partition coefficients (table 3.5.1) as well as concentration fractions in each environmental medium (table 3.5.2). In order to deal with temperature dependency, values for the enthalpy of phase change (ΔH) are presented along with the partition coefficients. Thus, partition coefficients can be deduced at any desired temperature by application of the Van 't Hoff equation: $\ln(K_2/K_1) = -\Delta H/R(1/T_2 - 1/T_1)$.

For inorganic mercury (and other metals), partition coefficients (among which specific values for marine waters) are provided by Crommentuijn *et al.* (1997). For elemental and organic mercury species, we calculated partition coefficient on the basis of the values, provided by Mackay (1996). To correct for the environmental temperature of 282 K, we used the Van't Hoff equation. The partition coefficients for partitioning between wet sediment an water, and between wet suspended matter and water, were calculated form the respective solid/water partition coefficients by assuming the volume ratio between water and solids to be 4 for sediment and 9 for suspended matter. The solid/water partition coefficient for soil was assumed to equal the corresponding sediment value. The volume ratio between solids and water was assumed to be 1 for soil, allowing for the calculation of separate soil/water partition coefficients. The aerosol/air

partition coefficients were calculated from the ratio between aerosol/water and air/water partition coefficients. The fraction of the chemical, associated to aerosols ($Fass_{aer}$) was calculated from these values to be 1.0 for each of the three mercury species. Values of the dimensionless partition coefficients calculated are shown in table 3.5.3

Table 3.5.1 Dimensionless partition coefficients K at 25° C and enthalpies of phase change ΔH (J·mol^{-1}) for the three groups of mercury species

	elemental Hg		inorganic Hg		organic Hg	
	K	ΔH	K	ΔH	K	ΔH
air/water	0.32	20 000	0.000001	30 000	0.30	30 000
aerosol/water	1 000 000	-5 000	10 000 000	-5 000	3 000 000	-5 000
sediment solids/water	20 000	-5 000	100 000	-5 000	5 000	-5 000
suspended solids/water	30 000	-5 000	200 000	-5 000	10 000	-5 000
fish/water	1	0	1 000	0	5 000 000	0

Source: Mackay *et al.*, 1995

Table 3.5.2 Concentration fractions of the three mercury species groups

	elemental Hg	inorganic Hg	organic Hg
input values			
air (vapor phase)	0.9998	0.0001	0.0001
water (dissolved phase)	0.020	0.900	0.080
sediment (solid phase)	0.010	0.980	0.010
fish (bulk fish)	0.020	0.020	0.960
calculated values			
aerosols	0.003	0.997	0.000
suspended solids	0.003	0.992	0.004
sediment pore woater	0.041	0.792	0.163
bulk phase			
air	0.980	0.020	0.000
water	0.014	0.933	0.053
sediment	0.010	0.980	0.010

Source: Mackay *et al.*, 1995

Table 3.5.3 Dimensionless partition coefficients used for the three groups of mercury species

	elemental Hg K[a]	inorganic Hg K[b]	organic Hg K[a]
air/water	2.0E-01	5.0E-07	1.5E-01
sediment/water	4.5E+03	5.61E+04	1.1E+03
sea sediment/sea water	4.5E+03	2.23E+04	1.1E+03
soil/water	9.0E+03	1.70E+02	2.2E+03
suspended matter/water	3.4E+03	4.25E+04	1.1E+03
sea suspended matter/seawater	3.4E+03	1.14E+04	1.1E+03
fish/water	1.0E+00	1.0E+03	5.0E+06

[a] Calcualted from: Mackay *et al.* (1995) (table 3.5.1 of this report)
[b] Calculated from K_p values, provided by Crommentuijn *et al.* (1997)

In order to make it possible to introduce mercury into the REIMSEA model without changing the model as such, a solution had to be found for the fact that the emission of one mercury species into the environment results in formation of three mercury species that differ with respect to both physico-chemical and toxicological properties. Weighted means were used for both toxicological values and partition coefficients. Partition coefficients for the three separate species were first calculated for each relevant phase change. As weighting factors, the ratios in which the three species occur in the 'departure medium' (table 3.5.2) were used. Since each phase change can take place in two directions, this would in theory deliver two separate partition coefficient for each couple of media between which direct exchange of chemicals can occur: one for each side. In the EUSES 1.00 model, however, for each couple of phase changes, calculations are base on the partition coefficient for only one of the two sides. (Air-water is the only exception, but there, air-water exchange is zero for mercury, due to the value of 1 for the fraction, associated to aerosols. Thus, only one air-water partition coefficient remains to be relevant for mercury.) Partition coefficients were calculated for these relevant direction only. Arithmetical means were calculated for those partition coefficients that appear in the numerators of the formulas, while harmonic means were calculated for those partition coefficients that appear in the denominators of these formulas. All values are specified and listed in table 3.5.4.

Table 3.5.4 Weighted means of dimensionless partition coefficients K at 9° C for each phase change (as far as relevant for the REIMSEA model)

	side	type of means	mean K
air/water	water	arithmetical	1.61E-02
sediment/water	sediment	harmonic	7.11E+03
sea sediment/seawater	sediment	harmonic	6.13E+03
soil/water	soil	harmonic	2.46E+01
suspended matter/water	water	arithmetical	3.84E+04
sea suspended matter/seawater	water	arithmetical	1.04E+04
fish/water	water	arithmetical	4.01E+05

Calculated from: Mackay *et al.*, 1995 (table 3.5.2 of this report) and table 3.5.3

3.6 Dissolved versus adsorbed

Natural waters are in fact mixtures of water and suspended matter. Most substances in the water compartment will be adsorbed to a greater or lesser extent to suspended particles. For aquatic toxicity assessment, we leave the adsorbed fraction out of consideration in our model. The ratio between adsorbed and dissolved species of metal ions in sea water depends on the concentration and nature of suspended particles, on the mutual forces between these particles on the one hand and each individual metal on the other, and on qualities of the solvent (e.g. fresh or salt water). Table 3.6.1 gives an overview of empirical partition coefficients between suspended matter and sea water, established for a number of metals in water of the North Sea and Wadden Sea. We have used these values for ocean water as well. Since the concentration of suspended matter in the North Sea is much higher than in the oceans, a relatively large part of the metals will exist in the adsorbed form in North Sea water. Only the dissolved fraction is assumed to cause toxic effects.

Table 3.6.1 Partition coefficients (logarithms) for metals between suspended matter and sea water, at different locations in the North Sea and Wadden Sea, in l/kg (Crommentuijn *et al.*, 1997)

metal	log K_p
Cadmium	4.23
Chromium	5.70
Copper	4.28
Lead	5.65
Mercury	4.66
Nickel	4.18
Zinc	5.04

3.7 Sedimentation and vertical mixing

In this report, the term 'sedimentation' is understood to refer to the gravitation-driven sinking of particles and adsorbed substances, whether or not these particles and substances eventually reach the sediment. Sedimentation in the surface mixed ocean layer thus refers to particle transport to the deep ocean layer, and not necessarily to the ocean sediment.

In the EUSES 1.00 model, the sedimentation rate of organics is modelled as a function of the suspended matter/water partition coefficient, the sedimentation rate of these particles as such, and the concentration of suspended particles. For sedimentation of organics in the surface mixed ocean layer, we have followed this same approach. For sedimentation in the North Sea, we adapted the approach by accounting for the specific deposition velocity in the North Sea, as described in chapter 2. We maintained the concept of the suspended matter/water partition coefficient as a basis for our calculations, however, both for organics and metals. For metal sedimentation in the surface mixed ocean layer, however, we developed a specific approach.

For metals, sedimentation in the surface mixed ocean layer is a key process.The surface mixed ocean layer functions as the environmental sink where the largest part of most undegradable substances will end up, before being immobilised by the one and only immobilisation process included in EUSES 1.00: sedimentation. The deep ocean is not considered as part of the environmental system. The sedimentation rate of metals in the surface mixed ocean layer thus largely determines the residence times of metals in the environmental system, and therewith eventually their LCA characterization factors.

Because of its key role, sedimentation in the surface mixed ocean layer should be modelled as accurately as possible. Deriving metal sedimentation rates from the combination of particle sedimentation rates and suspended matter/water partition coefficients, as mentioned above, is not fully satisfactory for this purpose. Suspended matter is a heterogeneous mixture of particles that largely differ in size and content, and therefore also in sedimentation rate and metal adhesion. Partition coefficients are average values, that do not reflect the specific adsorption of a metal to a specific kind of suspended matter. The particle sedimentation rate in the EUSES 1.00 model is also an average value, that does not reflect the specific sedimentation rate of different kinds of particles. Combining these average values may cause deviations between the calculated and actual sedimentation rates that – if applied to the ocean surface mixed layer – may eventually produce unrealistic LCA characterization values for metals. If possible, the use of empirical, metal-specific residence times for the estimation of sedimentation rates would be largely preferable.

Bruland (1980) gives an overview of mean residence times with respect to particulate removal of metals in a 80 m surface mixed layer of the North Pacific, estimated from measured concentrations and inputs by atmospheric fluxes and vertical mixing (table 3.7.1). Other sources of in- and output, such as eddy diffusion (or convection), and horizontal advection and diffusion, are stated to play a minor role within this oceanic region, and have been left out of consideration. We adapted these residence times for a 100 m surface mixed layer, assuming a constant mean net deposition rate, and used these adapted residence times for the calculation of advective flows from the surface mixed layer to the deep ocean.

Table 3.7.1 **Estimated atmospheric fluxes, net vertical mixing input fluxes, and mean residence times in surface mixed layer (80 m) with respect to particular removal of metals in the North Pacific(Bruland, 1980)**

metal	atmospheric input ($nmol \cdot cm^{-2}yr^{-1}$)	net vertical mixing input fluxes ($nmol \cdot cm^{-2}yr^{-1}$)	mean residence time (part. removal) [years]
Cadmium	0.0018	0.14	0.1
Copper	0.16	0.21	10
Lead	0.18	-0.01	3
Nickel	0.043	0.8	20
Zinc	0.40	0.15	1.0

4 SUBSTANCE CHOICE AND DATA

4.1 Selection of substances

Produced water, as it is being discharged from oil and gas producing platforms in the North Sea, is a complex mixture of water, organic and inorganic compounds. The exact composition of produced water varies from platform to platform, and for each platform the composition may vary in time. In general, however, a rough characterization of the produced water composition can be made. As a basis, a study performed by Slager *et al.* (1993) can be used, in which produced water from all producing platforms in the North Sea has been analysed and reported. The following table (4.1.1) shows the average composition of produced water.

Table 4.1.1 Overview of the composition of produced water. The second column shows the concentration of the chemicals (in $\mu g.l^{-1}$); the third column shows the relative toxicity of the components, expressed as Toxic Units. 'N.T.D.' means that no Toxic Units could be calculated.

Component	Median concentration [µg/l]	Relative toxicity [Toxic Units]
Oil**	190000	76.00
Benzene	74000	2.99
Toluene	6570	0.38
Ethylbenzene	340	0.04
Xylene	2300	0.31
Naphthalene	300	0.13
Biphenyl	140	<0.001
Fluorene	7.5	<0.01
Phenanthrene	7.25	0.01
Acenaphthene	63.5	<0.01
Acenaphthylene	59	N.T.D.
Fluoranthene	4.9	0.01
Anthracene	0.25	<0.01
Pyrene	1.05	N.T.D.
Benzo(a)pyrene	-	<0.01
Chrysene	-	<0.01
Benz(a)anthracene	-	<0.06
Perylene	-	<0.03
Benz(b)fluoranthene	-	N.T.D.
Benz(k)fluoranthene	-	<0.07
Dibenz(a,h)anthracene	-	<0.25
Benzo(ghi)perylene	-	<5
Indeno(1,2,3)pyrene	-	N.T.D.
Dibenzothiophene	-	-
Phenol	3700	0.28
Cresol	-	-
Xylenol	-	-
Glycol	125000	<0.01
Methanol	61000	0

25

**The total of aliphatic and aromatic hydrocarbons, measured according to NEN 6675 en NEN 6675 modified.

Component	Median concentration [µg/l]	Relative toxicity [Toxic Units]
Acetic acid	82000	N.T.D.
Propionic acid	11000	
Butanoic acid	7000	
Pentanoic acid	8000	
Hexanoic acid	6500	
Cadmium	50	0.08
Mercury	4.3	0.09
Lead	550	0.71
Zinc	14000	17.5
Arsenic	1.5	N.T.D.
Copper	25	0.13
Chromium	50	0.01
Nickel	45	0.01
Manganese	3300	N.T.D.
Barium	1790	0.28

Also shown in this table is the relative toxicity of each of the components, expressed as Toxic Units. On the basis of their concentration in produced water and the relative toxicity, a series of 18 components have been selected as relevant for modelling in the REIM-model. These components therewith cover all types of chemicals, present in produced water. The final selection in given in the following table.

Table 4.1.2 Overview of the substances selected as representative components of produced water, to be used in the REIM-model.

Selected substances
Benzene
Cadmium
Chromium
Ethylbenzene
Fluoranthene
Fluorene
Glycol
Lead
Mercury
Methanol
Naphthalene
Nickel
Oil
Phenanthrene
Phenol
Toluene
Xylene
Zinc

4.1.1 Production chemicals

Although not shown in the above tables, there might also be a discharge of production chemicals

with the produced water. Production chemicals are added to the system to enhance oil or gas production, protect the well or the equipment. Commonly used production chemicals are 'corrosion inhibitors', demulsifiers, scale inhibitors and anti foam agents. Some of these compounds have surface active properties (surfactants). It is, for as yet, not possible to model the fate of a surfactant in a multi-media model as applied in this study. In combination with the fact that the half-life time of surfactants is considerably low (usually in the order of 1-2 days) and that surfactants are likely to end up in the sediment with settling suspended matter, it has been decided to exclude surfactants from the current version of the model.

4.1.1.1 Organic acids

Table 4.1.1 shows that organic acids are present in produced water in relatively high concentrations. They have, however, not been included in the model since their toxicity is based upon the effects of lowering the pH. Since the buffering capacity of seawater will balance the change in pH, no adverse environmental effects are expected from the discharge of organic acids.

4.1.2 Toxicity threshold values

For the multi-media approach followed by REIMSEA, it is necessary to use toxicity threshold values for the aquatic ecosystem, terrestrial ecosystem and threshold values for human intake through food. Inverse threshold values are used as direct measures for the relative toxicity of substances in relation to each other in the calculation of characterization factors for toxic impacts (that are a function of toxicity, substance fate and exposure). The three types of toxicity threshold values used will be discussed separately in the following chapters.

4.1.3 Marine aquatic toxicity

The aquatic toxicity thresholds are used for defining equivalence factors for the environmental theme ecotoxicity. Since equivalence factors are a relative measure of toxicity, it is not important how the threshold is estimated, but even more important to represent the relative toxicity of the components. It has therefore been decided to use the geometric mean EC_{50} for each substance (as shown in Table 4.1.3). The EC_{50} values are derived from the TNO database *Medusa's Head*, which contains the results of toxicity experiments, as reported in scientific publications. Each EC_{50} in table may be based on data for several species, measuring the effect at different endpoints. To prevent the use of data for less relevant endpoints for this study (such as reduced enzyme activity or behavioural distortion), the selected data has been limited to effect-types related to mortality, growth and reproduction. From this data, the overall geometric mean has been calculated, and is presented in table 4.1.3.

By using the overall geometric mean, variation in toxicity due to the different species, effect types, life stages and exposure times is included in the one figure used in the REIM-model. On the one hand this introduces a substantial source for uncertainty, but on the other hand it reflects the situation that might occur in the field situation.

With respect to oil: since there is a large variation in the toxicity of oil, it is difficult to make a clear distinction between the toxicity of light and heavy oil types. Scholten et al., 1993, calculated the geometric mean EC50 of 12 different types of oil, showing lower toxicity for the lighter types of oil (EC50 of 4 mg/l for an average crude oil, vs. 20 mg/l for light crude and diesel). Furthermore, experimental studies lead to geometric mean EC50 values for condensate of 26 mg/l. These differences in toxicity appear to be caused by the fraction of C16-C22 components in the oil, causing physical effects such as smothering. It appeared that it is this fraction which is determining the actual toxicity of oil, and should be used as the fraction to standardise oil toxicity data (Evers et al, 1997).

It has to be noted that no distinction was made between freshwater data and seawater data. Previous, non-published, studies of TNO have shown that there is no substantial difference in the sensitivity of freshwater species and saltwater species. The variation introduced by this factor is insignificant in comparison with the sources of variation discussed above.

Table 4.1.3 Geometric mean of aquatic EC_{50} values [$\mu g.l^{-1}$]

Substance	Parameter value
Benzene	44812
Cadmium	553
Chromium	5601
Copper	
Ethylbenzene	18005
Phenanthrene	827
Phenol	17775
Fluoranthene	500
Fluorene	3671
Glycol	26213000
Mercury	47
Lead	645
Methanol	8944272
Naphthalene	2342
Nickel	2833
Oil	4000
Toluene	11924
Xylene	5716
Zinc	235

4.1.4 Freshwater aquatic toxicity

For freshwater aquatic toxicity, we used the aquatic Predicted No Effect Concentrations (PNECs), collected by Huijbregts (1999) for LCA-puposes, as effect factors.

Table 4.1.4 Aquatic Predicted No Effect Concentrations [kg.m^{-3}]

Substance	Parameter value
Benzene	$2.4 \cdot 10^{-3}$
Cadmium	$3.4 \cdot 10^{-7}$
Chromium	$3.4 \cdot 10^{-5}$
Copper	$1.1 \cdot 10^{-6}$
Ethylbenzene	$3.7 \cdot 10^{-4}$
Phenanthrene	$3.2 \cdot 10^{-6}$
Phenol	$9.0 \cdot 10^{-7}$
Fluoranthene	$2.4 \cdot 10^{-7}$
Fluorene	Na
Glycol	Na
Mercury	$\cdot 10^{-}$
Lead	$1.1 \cdot 10^{-5}$
Methanol	Na
Naphthalene	$4.2 \cdot 10^{-7}$
Nickel	$1.8 \cdot 10^{-6}$
Oil	Na
Toluene	$7.3 \cdot 10^{-4}$
Xylene	Na
Zinc	$6.6 \cdot 10^{-6}$

4.1.5 Terrestrial toxicity ($PNEC_{terrestrial}$)

One of the constraints of the REIM-model is to comply with the CHARM-model as much as possible. Since CHARM is limited to effects on marine organisms only, soil threshold values have been derived from '*Bouwstoffenbesluit bodem- en oppervlaktewaterenbescherming*' as being part of the '*Wet bodembescherming*'. The threshold values, as reported in the following table, are standardised on an organic matter content of 10 mg.kg^{-1} (dry matter) and a clay content of 25 mg.kg^{-1} (dry matter).

Table 4.1.5 Terrestrial ecological threshold values [mg.kg^{-1} dry matter]. 'na' means that no data exists for these substances; '(d)' means: equals detection limit.

Substance	Parameter value
Benzene	0.05 (d)
Cadmium	0.81
Chromium	100
Copper	36
Ethylbenzene	0.05 (d)
Phenanthrene	0.045
Phenol	0.05 (d)
Fluoranthene	0.015
Fluorene	Na
Glycol	Na
Mercury	0.32
Lead	86
Methanol	Na
Naphthalene	0.015
Nickel	35
Oil*	50
Toluene	0.05 (d)
Xylene	0.05 (d)
Zinc	140

4.1.6 Thresholds for human intake through food (RfDs)

As for terrestrial toxicity, CHARM does not take into account possible effect on humans due to the consumption of fish, milk or meat with increased levels of toxic chemicals. It has therefore been decided to use the values for Reference Doses (RfDs) for oral human intake (which are comparable to the WHO Acceptable Daily Intake values (ADIS)) of the selected chemicals. Most data used in this study have been derived from the on-line IRIS database. For copper, we used the WHO ADI value, and for benzene, naphthalene and phenanthrene values for the Tolerable Daily intake (TDI) (Vermeire, 1992).

Table 4.1.6 Reference Dose (RfD) [mg.kg body weigth^{-1}.day^{-1}]. 'na' means that no data exists for these substances.

Substance	Parameter value
Benzene	$4\ 10^{-4}$
Cadmium	$1\ 10^{-3}$
Chromium	1
Copper	$1.4\ 10^{-1}$
Ethylbenzene	0.1
Phenanthrene	$2\ 10^{-2}$
Phenol	0.6
Fluoranthene	$4\ 10^{-2}$
Fluorene	$4\ 10^{-2}$
Glycol	Na
Mercury	$3\ 10^{-4}$
Lead	$4\ 10^{-2}$
Methanol	0.5
Naphthalene	$5\ 10^{-5}$
Nickel	$2\ 10^{-2}$
Oil	13.6
Toluene	0.2
Xylene	2
Zinc	0.3

4.2 Fate parameters

The following paragraphs give an overview of the physicochemical parameters of the selected substances, necessary for modelling the fate of these substances in a multi-media model. Specific issues will be discussed for each of the parameters.

The major problem in collecting these data appeared to be the various metals in the produced water. Although measured as metal-ions, these ions usually cannot be described by fate-parameters. Except for toxicity, most physicochemical parameters are available for the various metal-salts. It is therefore that for some parameters special assumptions had to be made for metals.

Another problem occurred when collecting the various parameters for oil. Oil is not a single substance, but a complex mixture of chemicals. Oil, as measured in produced water, is in fact the concentration of oil dispersed in the produced water after discharge, while the hydrocarbon components in produced water are in fact components of oil dissolved in the water during the process of production. Since the solving of hydrocarbons components from the oil droplets into the water may be assumed to be insignificant, only the oil (as a mixture) needs to be evaluated in the model. For most parameters the average out of a range of parameter values have been selected, to be able to deal with oil as a single substance instead of a mixture.

The disadvantage of using the average value from a range is that, for example with biodegradation, the persistent components are assumed to be as biodegradable as the easy biodegradable components. To be on the safe side it would therefore be better to use the worst case values from the range. However, since LCA is focusing on the relative differences between chemicals, the worst case approach cannot be used and the best option therefore is to use the average figure from a range.

Finally, a remark has to be made about the parameters for xylene. Xylene is in fact a mixture of three isomers: *m*-xylene, *o*-xylene and *p*-xylene. It appeared, however, that the physicochemical

properties of these isomers are very much alike. It has therefore been decided to include xylene as a single chemical.

4.2.1 Molecular weight (MOLW)

The molecular weight of organic substances can easily be determined from their chemical structure. Concerning metals, a choice had to be made whether to regard the metal-salts (which have been brought into solution) or the metal-ion. Since the latter is the component found in produced water, and the component that might cause environmental effects; these will be considered in this study. The molecular mass of metal ions is thus the molar mass of the metal itself.

Table 4.2.1 Molecular weight of the selected substances in [g.mole^{-1}].

Substance	Parameter value
Benzene	78.1
Cadmium	112.4
Chromium	52.0
Ethylbenzene	106.2
Phenanthrene	178.2
Phenol	94.1
Fluoranthene	202.3
Fluorene	166.2
Glycol	62.1
Mercury	200.6
Lead	207.2
Methanol	32.0
Naphthalene	128.2
Nickel	58.7
Oil*	200
Toluene	92.1
Xylene	106.2
Zinc	65.4

** Since oil is a mixture of substances, there is no molecular weight of its own. The figure in this table is based on the average molecular weight of the components of an intermediate oil type (Evers* et al., *1997)*

4.2.2 Vapour pressure (VP)

Vapour pressure is a parameter that is used to predict the potential for volatilisation of the chemical. It is therefore extremely dependent of the temperature at the interface between air and the substance itself. For most of the chemicals considered in this study the temperature at which vapour pressure was determined was 20 °C. If no data for this temperature could be found, data at a deviating temperature was reported.

Vapour pressure is not a relevant parameter for the metal-ions, and are therefore not reported.

In the original literature and databases vapour pressure was often expressed in millimetre mercury pressure (mm Hg). These data have been transformed into figures expressed as Pascal (Pa) by multiplication of the vapour pressure with a conversion factor of $1.33.10^2$.

For (intermediate) oil an evaporation rate of 0.113 d^{-1} was reported in Evers *et al.* (1997).

Table 4.2.2 Vapour pressure of the selected substances in [Pa]. 'na' means that no data exists for these substances.

Substance	Parameter value	Temperature of determination
Benzene	10108	20 °C
Cadmium	Na	
Chromium	Na	
Ethylbenzene	944.3	20 °C
Phenanthrene	0.0904	20 °C
Phenol	26.6	20 °C
Fluoranthene	0.000133	20 °C
Fluorene	1.729	20 °C
Glycol	0.082	20 °C
Mercury	Na	
Lead	Na	
Methanol	13300	21.2 °C
Naphthalene	6.65	25 °C
Nickel	Na	
Oil	26150	20 °C (Koops, 1992)
Toluene	2979.2	20 °C
Xylene	815.7	20 °C
Zinc	Na	

4.2.3 Water solubility (SOL)

The solubility of a chemical in water is a parameter that is rather generally available. Since the solubility of a substance in water is dependent of the temperature, all reported data is measured at 20 °C. There is also a reported difference between the solubility of a chemical in freshwater and the solubility in saltwater (Spriensma, 1995). Spriensma reported lower solubilities for BTXs in saltwater, but did not give a quantification. For C6-C10 alkanes the author reported 5 times higher solubility in saltwater relative to freshwater. Since no other data could be found to support these differences in solubility, data reported for this study are all based on freshwater.
The solubility of metals is fully dependent on the metal-salt used to bring the ions into solution. For the ions as such no solubility can be determined, and are therefore reported as 'na'.
Furthermore, it is also possible that there is no upper limit for the solubility of a chemical in water. These cases (glycol and methanol) have been reported as '>>'.

Table 4.2.3 Water solubility of the selected substances in [g.l^{-1}]. 'na' means that no data exists for these substances. '>>' means that no upper limit was reported for water solubility.

Substance	Parameter value
Benzene	1.78
Cadmium	Na
Chromium	Na
Ethylbenzene	$1.52\ 10^{-1}$
Phenanthrene	$1.6\ 10^{-3}$
Phenol	$8.28\ 10^{-1}$
Fluoranthene	$2.18\ 10^{-4}$
Fluorene	$1.8\ 10^{-3}$
Glycol	>>
Mercury	Na
Lead	Na
Methanol	>>
Naphthalene	$2.16\ 10^{-2}$
Nickel	Na
Oil*	$9\ 10^{-7}$ to $5\ 10^{-3}$
Toluene	$5.26\ 10^{-1}$
Xylene	$1.74\ 10^{-1}$
Zinc	Na

** Since oil is a mixture of substances, which varies between the different types of oil, solubility was reported as a range.*

4.2.4 Octanol-water partitioning (Kow)

Octanol-water partitioning coefficients (P_{ow} or K_{ow}) are reported for all organic chemicals. For metals, no K_{ow} can be determined (reported as 'na').

Data usually reported in databases and literature do not explicitly state the method used for determination, while this might be important for the actual reported figure. The original test for determining the K_{ow} is the OECD 107 (shake flask) test. In this test the chemical is added to equal amounts of octanol and water. After shaking the bottle the chemical dissolves in both the water- and the octanol-phase. The ratio between the concentrations in both phases is called the K_{ow}. Currently however, the OECD 117 (HPLC) test is used more often. In this test the retention time of a substance over a HPLC is correlated with the retention time of a set of standards with a known K_{ow}. This gives an (accurate) estimation of the K_{ow} of the substance.

In the CHARM-model data derived from the OECD 117 (HPLC) method is preferred above the data derived OECD 107 test. The latter are therefore used with a safety factor (log K_{ow} + 2) to account for the uncertainties in the OECD 107 test. *Data reported in this paragraph do* ***not*** *include this safety factor, but to stay in line with the CHARM-model the use of this safety factor could be considered.*

It must be noted that the usual notation of the octanol-water partitioning coefficient is the **log** K_{ow}. This is also the notation used in this study.

Table 4.2.4 Logarithm of the octanol-water partitioning coefficient of the selected substances [-]. 'na' means that no data exists for these substances.

Substance	Parameter value
Benzene	2.13
Cadmium	na
Chromium	na
Ethylbenzene	3.15
Phenanthrene	4.46
Phenol	1.46
Fluoranthene	5.16
Fluorene	4.18
Glycol	-1.36
Mercury	na
Lead	na
Methanol	-0.77
Naphthalene	3.3
Nickel	na
Oil*	6.3
Toluene	2.73
Xylene	3.01
Zinc	na

** Since oil is a mixture of substances, it cannot be characterized by a K_{ow}. The figure in this table is therefore derived from the K_{oc} of an intermediate type of oil (Ewers et al., 1997).*

4.3 Melting point (TEMPmelt)

The melting point is a standard parameter for the organic chemicals. Concerning metals it is only the salts for which a melting point can be determined. The parameter is not available for the metal-ions.

Table 4.3.1 Melting point of the selected substances in [°C]. 'na' means that no data exists for these substances.

Substance	Parameter value
Benzene	5.5
Cadmium	Na
Chromium	Na
Ethylbenzene	-95
Phenanthrene	99.5
Phenol	40.5
Fluoranthene	110.8
Fluorene	116
Glycol	-13
Mercury	Na
Lead	Na
Methanol	-98
Naphthalene	80.6
Nickel	Na
Oil*	-38 - +96
Toluene	-93
Xylene	-50
Zinc	Na

** Since oil is a mixture of substances which varies between the different types of oil, the melting point is reported as a range, determined from the melting point of the individual constituents.*

4.3.1 Henry's law constant (HENRY)

No difficulties were encountered while searching for the Henry's law constant. Again, for metal-ions no parameter values can be reported. The original data was expressed as mole per atmosphere ($M.atm^{-1}$). These data have been transformed such that they could be expressed as $Pa.m^3.mole^{-1}$, by taking the reciprocal of: the original figure multiplied by 101.325:

Table 4.3.2 The reciprocal value of the Henry's law constant of the selected substances in [$Pa.m^3.mol^{-1}$]. 'na' means that no data exists for these substances.

Substance	Parameter value
Benzene	506.63
Cadmium	Na
Chromium	Na
Ethylbenzene	779.42
Phenanthrene	3.4940
Phenol	0.04053
Fluoranthene	220.27
Fluorene	9.2114
Glycol	0.0059603
Mercury	Na
Lead	Na
Methanol	0.46057
Naphthalene	48.25
Nickel	Na
Oil	100
Toluene	633.28
Xylene	605.14
Zinc	Na

4.3.2 Dissociation constant (pKa)

This parameter is to be used for only a few of the selected chemicals: phenol and glycol, the other chemicals are not subject to dissociation. The respective parameter values for these compounds are $1.28\ 10^{-10}$ and $6.00\ 10^{-15}$ (at 20°C). Because of the extremely small dissociation constant for these compounds, it has been decided to exclude dissociation processes from the model.

4.3.3 Photodegradation ($DT_{50}photo_{air}$)

Photodegradation is an important parameter for volatile chemicals. Once available in a gaseous form in the air, the molecules might be degraded due to exposure by sunlight. This process is quantified by the parameters in the following table:

Table 4.3.3 Half-life for photodegradation in air [hours]. 'na' means that no data exists for these substances.

Substance	Parameter value
Benzene	275.6
Cadmium	Na
Chromium	Na
Ethylbenzene	47.1
Phenanthrene	11.1
Phenol	12.5
Fluoranthene	11.1
Fluorene	37.5
Glycol	45.7
Mercury	Na
Lead	Na
Methanol	392
Naphthalene	16.3
Nickel	Na
Oil	Na
Toluene	57.0
Xylene	23.1
Zinc	Na

4.3.4 Hydrolysis (DT50hydro)

None of the selected substances have hydrolysable groups. Hydrolysis is therefore not a relevant parameter in this model.

4.3.5 Biodegradation in water

Biodegradation is an important process in the water phase, and can for each substance be quantified by the degradation half-life time. Since the biodegradation products are not regarded in the model used for this study, it leads to a loss of chemicals from the system.

Table 4.3.4 Biodegradation half-life time of the selected substances [hours] in freshwater. 'na' means that no data exists for these substances.

Substance	Parameter value
Benzene	252
Cadmium	Na
Chromium	Na
Ethylbenzene	156
Phenanthrene	2592
Phenol	45
Fluoranthene	6960
Fluorene	1104
Glycol	168
Mercury	Na
Lead	Na
Methanol	96
Naphthalene	246
Nickel	Na
Oil*	146
Toluene	312
Xylene	420
Zinc	Na

** Since oil is a mixture of substances, its half-life is fully dependent on the individual substances. More persistent components will dominate in the oil after some time of degradation. The figure in this table is derived from Evers* et al. *(1997) and represents an intermediate type of oil.*

4.3.6 Biodegradation in soil

In most cases biodegradation half-life time in soil is assumed equal to the biodegradation half-life time in water. In two cases (phenol and naphthalene), however, specific experiments have been carried out to come up with an accurate figure for the half-life time in soil.

Table 4.3.4 Half-life time of the selected substances [hours] in soil. 'na' means that no data exists for these substances.

Substance	Parameter value
Benzene	252
Cadmium	Na
Chromium	Na
Ethylbenzene	156
Phenanthrene	2592
Phenol	132
Fluoranthene	6960
Fluorene	1104
Glycol	168
Mercury	Na
Lead	Na
Methanol	96
Naphthalene	775
Nickel	Na
Oil*	146
Toluene	312
Xylene	420
Zinc	Na

** Since oil is a mixture of substances, its half-life is fully dependent on the individual substances. More persistent components will dominate in the oil after some time of degradation. The figure in this table is derived from Evers et al. (1997) and represents an intermediate type of oil.*

4.3.7 Bioconcentration (BCF)

Bioconcentration factors for metals were taken from Huijbregts (1999). For organics, the model contains an estimation routine for bioconcentration factors.

Table 4.3.5 Bioconcentration factors (marine organisms) of the selected metals [l.kg^{-1} wet weight].

Substance	Total
Cadmium	38
Chromium	40
Copper	120
Mercury	4524
Lead	500
Nickel	87
Zinc	1000

4.3.8 Bioconcentration in plant leaves

Although not available in the same quantities, a set of bioconcentration data could be derived for plants as well. The figures in the following table represent the accumulation of chemicals from the soil into the stem and leaves of the plant. Since the BCF can be calculated on the basis of the log K_{ow} as well, this parameter was only obtained for metals (table 4.3.7).

Table 4.3.6 Bioconcentration factors (plant leaves) of the selected metals [mg.kg ds^{-1}].[mg.kg ds^{-1}]$^{-1}$.

Substance	Total
Cadmium	0.15
Chromium	0.002
Mercury	0.015
Nickel	0.07
Lead	0.001
Zinc	0.1

4.3.8.1 Bioconcentration in cattle meat and milk

Data for bioconcentration of the substances in cattle milk and meat could hardly be found in the available literature and databases. For organic substances these data can be estimated using their K_{ow}. Since this is not possible for metals, their BCF values have been derived from single literature reference.

Table 4.3.7 Bioconcentration factors for cattle meat and milk (metals only) Respective units: [d.kg^{-1}] and [d.L^{-1}].

Substance	BCF meat	BCF milk
Cadmium	$7.2\ 10^{-4}$	$1.5\ 10^{-3}$
Chromium	$9.2\ 10^{-3}$	$1.1\ 10^{-3}$
Mercury	$7.1\ 10^{-3}$	$4.7\ 10^{-4}$
Lead	$1.0\ 10^{-4}$	$2.6\ 10^{-4}$
Nickel	$2.0\ 10^{-3}$	$1.0\ 10^{-3}$
Zinc	$1.2\ 10^{-1}$	$1.0\ 10^{-2}$

4.3.9 Solids-water partitioning

For organic chemicals the solid-water partitioning can be calculated on the basis of the organic matter content of the solid phase and their lipophility (expressed as the K_{ow}). For metals, however, this is a figure that has to be derived experimentally. The soil-water partitioning coefficients of metals are, however, dependent upon the type of soil. The figures presented in Table 4.3.9, have therefore been calculated as weighted average of the different types of soil. Weighing factors were based upon the relative abundance of the individual soil types in the Netherlands (50% sand, 40% clay and 10% peat). The following table shows the soil-water partitioning for metals:

Table 4.3.8 Partitioning between water and soil (Kd) of the selected substances [l.kg^{-1}].

Substance	Parameter value
Cadmium	1940
Chromium	33120
Mercury	5600
Lead	14020
Nickel	1700
Zinc	1890

Comparable to the solids-water partitioning, the same parameter can be derived for partitioning between water and suspended matter. For determining these figures the suspended matter did only include clay particles (while in seawater organic matter and algae are also part of the suspended matter).

Table 4.3.9 Partitioning between water and suspended matter (Kd) of the selected substances [$L.kg^{-1}$].

Substance	Parameter value
Cadmium	$5\ 10^3$
Chromium	$5\ 10^4$
Mercury	$5\ 10^3$
Lead	$3\ 10^7$
Nickel	$1\ 10^6$
Zinc	$2\ 10^5$

5 CHARACTERIZATION

5.1 Introduction

EUSES 1.00 has not been developed for LCA-purposes: it is a risk evaluation model. Especially in the effect assessment there are important differences between LCA and risk assessment. One of the main goals of risk assessment is, to design environmental standards for toxic substances. To prevent toxic effects, standards should rather be too severe than too mild. To prevent high societal costs and erroneous political priorities, however, standards should not be more severe than necessary. For these reasons, environmental standards are often based on a worst-case approach for each individual substance. The more information on a substance is lacking, the larger the safety margin should be in order to be 'at the safe side'. Safety margins can be obtained either by the application of safety factors, or by the use of extreme default values. Safety factors are often being applied to uncertain toxicity data, used for effect assessment. In relation to fate analysis, especially the use of extreme default values is interesting. Extreme default values are sometimes applied where specific substance-data are lacking. They are chosen extreme 'in the safe direction', which means they are either high or low, depending on the way they influence the standard to be designed.

Although the use of substance-specific safety margins may be a very valuable compensation for uncertainty in risk assessment, their use in LCA is not appropriate, and can easily give rise to erroneous results. In LCA, it is not standards, but characterization factors that play a central role. The ratios between the characterization factors for toxicity of two different substances are intended to reflect the ratios between the amounts of 'potential toxicity', introduced into the environment by equal amounts of these substances. Safety margins for individual substances – either applied in fate analysis or in effect assessment – may easily disturb these ratios. For lacking substance data, this implies that a 'best guess' is preferred to the use of an extreme default value. If the use of a default value is inevitable, this default should be based on an average – rather than an extreme – value. The characterization factor of each substance should represent its most probable harmfulness, compared to other substances. The use of 'pure' (experimental) toxicity data is therefore favoured above the use of standards, in which ratio-disturbing safety factors may be included. Characterization factors should remain as close as possible to basic impact information. Extrapolations (e.g. from LC_{50} to NOEC) should be based on probabilities, not on worst case assumptions and safety factors.

In this report, only toxic substances are considered. As ecotoxicity factors, EC_{50} values were used for marine ecotoxicity as far as possible. For human toxicity, values for the oral *reference dose* (RfD) and the inhalatory *tolerable concentration in air* (TCL) were used.

5.2 The nature of toxicity characterization factors

In EUSES 1.00, *risk characterization ratios* (RCRs) for ecotoxicity are calculated as the ratio between the *predicted environmental concentration* (PEC), calculated with the multimedia model, and the *predicted no effect concentration* (PNEC), which is calculated from toxicity data to which the appropriate safety margins have been applied. An ecotoxicity RCR above 1 indicates that the environmental threshold has been surpassed by the predicted average concentration. In life cycle ecotoxic impact assessment, an equivalent procedure is used, but with different parameters, and for a different goal.

In LCA, there is no PEC. The emissions to be assessed in LCA are not continuous, but are expressed

as amounts, emitted in relation to a functional unit, over an unspecified time span. While the common use of multimedia models is the calculation of (usually steady-state) concentrations, these same models are used in LCA for the calculation of amounts of substance, present in each compartment, integrated over an infinite time span. These amounts are proportional to the emitted amount and of the compartment volume, and are functions of degradation and immobilisation rates and intercompartmental transport parameters. Intercompartmental transport can take place either between different media within a region or between equivalent media in different regions. Contrary to the environmental concentrations calculated in steady state models, these time-integrated amount are independent of the emission rate; it is only the amount emitted that is decisive. For this reason, it is not possible to talk about either or not surpassing threshold values on the basis of common LCA data.

The goal of the characterization is the aggregation of emissions of different substances to different environmental compartments in different regions to one overall impact score per impact category. Time integrated environmental amounts of different substances are weighted against each other by their relative toxicity. Toxicity threshold values, such as NOECs, EC_{50}s and LC_{50}s can be used for this purpose. In order to translate different kinds of toxicity data into one uniform type, safety margins have sometimes been used, and the result of this procedure has sometimes been called PNEC. The subsequent procedure, where predicted environmental amounts are divided by these 'PNECs' seems to be almost similar to the ecotoxicity RCR procedure in risk assessment. While this last procedure is used to assess whether thresholds have been surpassed or not, however, the LCA-procedure is used to weight amounts of different substances against each other, so that they can be aggregated into one impact score per impact category. Ecotoxicity characterization factors are factors, calculated according to this procedure, per unit emission to a certain environmental compartment. Multiplication of the characterization factor with the actual emission, expressed in the same unit, delivers the impact score per substance and per emission compartment for each impact category. Eventually, all impact scores are summed to one overall impact score per impact category.

For human toxicity, an equivalent procedure is used, but an intake module is added to account for differences in intake, due to intake routes via different environmental compartments: air, water and agricultural soil (via crops). Eventually, the results can also be summed into one overall impact score for human toxicity, aggregated over all substances and compartments.

The inclusion of multimedia transport results in a distribution of any emission over all environmental compartments. For this reason, aquatic toxicity is not only caused by emissions to water, but also by emissions to air or soil. Every emission will therefore have an characterization factor for all four ecotoxicity impact categories considered in this report, instead of only one, as it used to. Including fate thus inevitably lead to a multiplication of the number of characterization factors. The same applies to the use of a regionalized approach. In this report, where four environmental regions are distinguished (North Sea, The Netherlands, the world continents and the world oceans), each substance can be emitted to 16 different environmental compartments. Since each of these emissions is characterised by its own specific contributions to each of the four toxic impact categories considered, this results in 64 characterization factors per substance. All (eco)toxicity characterization factors, with directions for use, are listed in appendix A. The impact scores, calculated with these characterization factors, are of dimension *days* (human toxicity) and *days* $\times m^3$ (ecotoxicity). For human toxicity, this results can artificially be imagined to correspond to the number of seconds that humanity, due to the emission at stake, could be exposed to a level that corresponds to the ADI, TDI OR TCL value. For ecotoxicity, the result can be imagined to correspond to the number of secnds that the ecosystem at stake would be exposed to a level that corresponds

to the NOEC or EC_{50} value applied.

5.3 Nutrification

Some of the compounds used in the off shore industry can contribute to the problem of nutrification. In the framework of this project, no specific modelling has been performed for these nutrification potentials. It is recommended to use the nutrification potentials (NP) which are given in the 2002 LCA Guide (Guinée, 2002). These characterization factors are related to PO_4^{3-}, which has a NP of 1.00. For the sum-parameter Chemical Oxygen Demand (COD), a value of 0.022 is given. The COD of a compound can be measured, but here it is calculated on the basis of the amount of O_2 that is needed to oxidise the compound under consideration.

6 DISCUSSION

One of the most innovative features of this project is the inclusion of metals in a fate model with a metal-specific approach, accounting for speciation and for specific behaviour with respect to sedimentation. The complex behaviour of mercury has also been taken into account, without affecting the relative simplicity of the multimedia model. Unless all these accomplishments, it turns out that the differences in characterization factors between metals and organics remain very large, unless exposure via the ocean is not accounted for. If the oceanic exposure route is taken into account, metal emissions will easily dominate emission profiles. This phenomenon is caused by the fact that metals are non-degradable. The only way by which they can leave the system is sedimentation. Since specific sedimentation rates have been introduced for most individual metals, the very high residence times of metals in the environmental system cannot be considered merely as model artefacts. Rather, they raise the question whether the LCA approach to assess the anthropogenic environmental presence of substances merely on the basis of amounts, independent of the environmental concentrations, caused by these amounts, always makes sense. It may be argued that as long as total anthropogenic emission levels of a substance do not considerably add to the natural background in a certain compartment, or – alternatively – as long as concentrations remain far below environmental no effect levels, direct or indirect emissions to this compartment could be left out of consideration. Although this seems to be an attractive and sensible option, it should, in practice, be handled with great care. Multimedia models presume homogeneous concentrations and instantaneous dilution of emitted substances. Increased concentrations around emission sources remain invisible, and even increased concentrations in large areas may be averaged out by lower concentrations elsewhere in the same compartment. The fact that a certain environmental threshold is not surpassed on an average basis – as pointed out by the result of multimedia modelling application – does not imply that this threshold is not surpassed on a local level. Considerable effects may occur without being recognised by multimedia modelling alone. Further research is needed in order to enable a more specific approach that leaves out those emissions that cause no harm at all, but that maintains – possibly in an adapted form – the assessment of emissions that cause local effects.

Another aspect that needs further research is toxic exposure- and effect modelling. This subject is beyond the scope of fate modelling; it is just another necessary component of LCA impact assessment modelling, which is – contrary to fate modelling – specific for toxicity impact. Possible extensions include the addition of more categories of ecosystem types, the refinement of exposure modelling for aquatic ecosystems and the refinement of human effect modelling. Ecosystem categories that could be added include sediment dwellers, birds, and mammals. With respect to the exposure of aquatic ecosystems, it could be investigated whether the direct relationship between concentration and ecotoxic effects on the basis of NOEC and EC_{50} values reflects long-term toxic effects well enough. Explicit exposure modelling may be more appropriate, but for LCA-purposes, such model should not be too specific. Preferably, one general exposure model should cover the entire aquatic ecosystem. A refinement of human toxicity modelling could encompass a distinction between different types of toxic effects, including their relative weights compared to each other.

As a whole, the REIMSEA model has surpassed the goal of merely adapting current LCA multimedia modelling to the local situation of the North Sea. With the introduction of specific adaptations to introduce metals in multimedia models, a step forward has been made in the

scientific state of the art. It should be kept in mind, however, that this is but a first step, that should be followed by many others.

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Appendix A CHARACTERIZATION FACTORS

Directions for use

1. Choose between the options *include all exposure routes* and *exclude exposure via ocean.* (This last option has been added to facilitate the analysis of the relative influence of exposure of man and marine ecosystems via the oceanic system, especially in case of emissions to the North Sea system.)
2. Specify each emission with respect to:
   - substance
   - emission region:
     one of the regions *North Sea, ocean ('atlantic'), The Netherlands ('regional')* and *world continents ('continental')*
   - emission compartment (one of the compartments *air, water, suspended matter* ('susp'), *seawater, sea suspended matter* ('seasusp'), *natural soil* ('nat') *industrial soil* ('ind'), and *agricultural soil* ('agr'))
   - amount (in tonnes)

   NB: Insoluble emissions to water should be entered as emissions to the suspended matter compartment.
3. Multiply each emission by the characterization factor that corresponds to the emission region and the emission compartment **for all four impact categories.**
   This should result in four impact scores **for each emission.**
4. Sum the impact score per impact category over all regions and all compartments for each substance.
   This should result in four impact scores **for each substance**: single scores for human toxicity, freshwater ecotoxicity, seawater ecotoxicity and terrestrial ecotoxicity.
5. Sum the impact scores per impact category over the different substances.
   This should deliver the final result: **four overall impact scores** for all emissions. together.

The summations in steps 3 and 4 can also be replaced by one overall summation.

Characterization factors for human toxicity, freshwater and marine aquatic ecotoxicity, and terrestrial ecotoxicity, per substance and emission compartment (all in $s \cdot kg^{-1}$)

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
benzene	regional, air	1.49E-08	1.18E-07	3.33E-02	5.66E-11	3.33E-02	5.43E-12
benzene	regional, water	5.17E-06	8.82E-08	2.96E-02	1.96E-10	2.96E-02	1.49E-10
benzene	regional, susp	4.74E-06	8.10E-08	2.72E-02	1.84E-10	2.72E-02	1.41E-10
benzene	regional, nat	4.83E-08	2.67E-05	2.90E-02	5.04E-11	2.90E-02	5.72E-12
benzene	regional, agr	3.55E-08	7.82E-05	4.60E-02	3.70E-11	4.60E-02	4.20E-12
benzene	regional, ind	4.83E-08	2.67E-05	2.90E-02	5.04E-11	2.90E-02	5.72E-12
benzene	continental, air	1.68E-08	1.32E-07	2.73E-02	4.80E-11	2.73E-02	2.48E-13
benzene	continental, water	5.99E-06	1.10E-07	2.33E-02	5.94E-11	2.33E-02	2.40E-13
benzene	continental, susp	5.96E-06	1.09E-07	2.32E-02	5.97E-11	2.32E-02	2.41E-13
benzene	continental, nat	5.54E-08	2.67E-05	2.38E-02	4.20E-11	2.38E-02	2.16E-13
benzene	continental, agr	4.07E-08	7.82E-05	1.82E-02	3.08E-11	1.82E-02	1.59E-13
benzene	continental, ind	5.54E-08	2.67E-05	2.38E-02	4.20E-11	2.38E-02	2.16E-13
benzene	north sea, air	1.28E-08	1.01E-07	2.20E-02	6.76E-11	2.20E-02	1.08E-11
benzene	north sea, seawater	2.60E-09	2.05E-08	4.46E-03	1.02E-09	4.46E-03	9.52E-10
benzene	north sea, seasusp	2.60E-09	2.05E-08	4.46E-03	1.02E-09	4.46E-03	9.51E-10
benzene	atlantic, air	3.88E-09	3.06E-08	6.32E-03	1.13E-10	6.32E-03	9.63E-14
benzene	atlantic, seawater	7.53E-10	5.94E-09	1.23E-03	1.05E-09	1.23E-03	9.91E-14
benzene	atlantic, seasusp	7.53E-10	5.94E-09	1.23E-03	1.05E-09	1.23E-03	1.19E-13
cadmium	regional, air	8.50E-02	2.01E-04	5.87E+00	3.44E-07	5.87E+00	9.39E-09
cadmium	regional, water	3.16E-02		3.24E-03	2.54E-07	3.24E-03	2.12E-08
cadmium	regional, susp	2.89E-02		2.97E-03	2.47E-07	2.97E-03	2.06E-08
cadmium	regional, nat	1.58E-02	1.20E-04	1.62E-03	1.27E-07	1.62E-03	1.06E-08
cadmium	regional, agr	1.58E-02	4.80E-04	8.48E-01	1.27E-07	8.48E-01	1.06E-08
cadmium	regional, ind	1.58E-02	1.20E-04	1.62E-03	1.27E-07	1.62E-03	1.06E-08
cadmium	continental, air	1.11E-01	2.45E-04	4.24E+00	2.45E-07	4.24E+00	6.16E-10

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
cadmium	continental, water	2.75E-01		2.71E-03	1.57E-07	2.71E-03	3.27E-10
cadmium	continental, susp	2.74E-01		2.69E-03	1.56E-07	2.69E-03	3.27E-10
cadmium	continental, nat	1.38E-01	1.20E-04	1.35E-03	7.84E-08	1.35E-03	1.64E-10
cadmium	continental, agr	1.38E-01	4.80E-04	1.82E-02	7.84E-08	1.82E-02	1.64E-10
cadmium	continental, ind	1.38E-01	1.20E-04	1.35E-03	7.84E-08	1.35E-03	1.64E-10
cadmium	north sea, air	6.53E-02	1.45E-04	2.76E+00	4.62E-07	2.76E+00	1.80E-08
cadmium	north sea, seawater			3.68E-09	8.00E-07	1.05E-09	6.67E-08
cadmium	north sea, seasusp			3.68E-09	7.99E-07	1.05E-09	6.67E-08
cadmium	atlantic, air	8.23E-03	1.82E-05	3.15E-01	7.07E-07	3.15E-01	1.09E-09
cadmium	atlantic, seawater			2.69E-09	7.44E-07	1.76E-11	1.11E-09
cadmium	atlantic, seasusp			2.69E-09	7.44E-07	1.76E-11	1.12E-09
chromium	regional, air	4.08E-04	1.62E-06	2.84E-05	7.61E-12	2.84E-05	1.66E-13
chromium	regional, water	1.52E-04		1.56E-06	1.85E-12	1.56E-06	1.49E-13
chromium	regional, susp	1.40E-04		1.43E-06	1.78E-12	1.43E-06	1.43E-13
chromium	regional, nat	7.62E-05	9.73E-07	7.82E-07	9.26E-13	7.82E-07	7.44E-14
chromium	regional, agr	7.62E-05	3.89E-06	8.48E-04	9.26E-13	8.48E-04	7.44E-14
chromium	regional, ind	7.62E-05	9.73E-07	7.82E-07	9.26E-13	7.82E-07	7.44E-14
chromium	continental, air	5.32E-04	1.98E-06	8.14E-06	5.73E-12	8.14E-06	1.18E-14
chromium	continental, water	1.32E-03		1.30E-06	2.87E-12	1.30E-06	4.49E-15
chromium	continental, susp	1.32E-03		1.29E-06	2.86E-12	1.29E-06	4.48E-15
chromium	continental, nat	6.61E-04	9.73E-07	6.50E-07	1.43E-12	6.50E-07	2.24E-15
chromium	continental, agr	6.61E-04	3.89E-06	1.75E-05	1.43E-12	1.75E-05	2.24E-15
chromium	continental, ind	6.61E-04	9.73E-07	6.50E-07	1.43E-12	6.50E-07	2.24E-15
chromium	north sea, air	3.14E-04	1.18E-06	6.98E-06	1.01E-11	6.98E-06	3.28E-13
chromium	north sea, seawater			7.01E-16	1.51E-11	1.94E-16	1.22E-12
chromium	north sea, seasusp			7.00E-16	1.51E-11	1.94E-16	1.22E-12
chromium	atlantic, air	3.95E-05	1.47E-07	6.07E-07	1.78E-11	6.07E-07	2.46E-14
chromium	atlantic, seawater			6.87E-16	1.88E-11	4.04E-18	2.53E-14

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
chromium	atlantic, seasusp			6.86E-16	1.88E-11	4.04E-18	2.53E-14
copper	regional, air	5.67E-02	4.51E-06	1.75E-01	3.17E-06	1.75E-01	8.12E-08
copper	regional, water	2.08E-02		4.94E-05	2.91E-06	4.94E-05	2.42E-07
copper	regional, susp	1.91E-02		4.53E-05	2.78E-06	4.53E-05	2.32E-07
copper	regional, nat	1.04E-02	2.70E-06	2.47E-05	1.45E-06	2.47E-05	1.21E-07
copper	regional, agr	1.04E-02	1.08E-05	6.06E-03	1.45E-06	6.06E-03	1.21E-07
copper	regional, ind	1.04E-02	2.70E-06	2.47E-05	1.45E-06	2.47E-05	1.21E-07
copper	continental, air	7.39E-02	5.50E-06	1.27E-01	2.40E-06	1.27E-01	5.77E-09
copper	continental, water	1.84E-01		4.18E-05	2.13E-06	4.18E-05	4.16E-09
copper	continental, susp	1.83E-01		4.15E-05	2.12E-06	4.15E-05	4.15E-09
copper	continental, nat	9.19E-02	2.70E-06	2.09E-05	1.06E-06	2.09E-05	2.08E-09
copper	continental, agr	9.19E-02	1.08E-05	1.41E-04	1.06E-06	1.41E-04	2.08E-09
copper	continental, ind	9.19E-02	2.70E-06	2.09E-05	1.06E-06	2.09E-05	2.08E-09
copper	north sea, air	4.36E-02	3.27E-06	8.26E-02	4.10E-06	8.26E-02	1.52E-07
copper	north sea, seawater			9.20E-11	6.75E-06	2.63E-11	5.63E-07
copper	north sea, seasusp			9.20E-11	6.75E-06	2.62E-11	5.63E-07
copper	atlantic, air	5.49E-03	4.09E-07	9.45E-03	6.00E-06	9.45E-03	9.29E-09
copper	atlantic, seawater			6.72E-11	6.29E-06	4.39E-13	9.42E-09
copper	atlantic, seasusp			6.72E-11	6.29E-06	4.39E-13	9.43E-09
ethylbenzene	regional, air	1.27E-08	1.66E-08	2.85E-05	7.98E-12	2.85E-05	4.07E-12
ethylbenzene	regional, water	3.05E-05	1.13E-08	3.93E-05	2.38E-10	3.93E-05	2.27E-10
ethylbenzene	regional, susp	2.80E-05	1.04E-08	3.60E-05	2.25E-10	3.60E-05	2.15E-10
ethylbenzene	regional, nat	1.50E-07	1.78E-05	2.47E-05	7.95E-12	2.47E-05	4.54E-12
ethylbenzene	regional, agr	1.08E-07	5.12E-05	1.88E-04	5.72E-12	1.88E-04	3.26E-12
ethylbenzene	regional, ind	1.50E-07	1.78E-05	2.47E-05	7.95E-12	2.47E-05	4.54E-12
ethylbenzene	continental, air	1.61E-08	2.06E-08	1.42E-05	3.08E-12	1.42E-05	4.72E-14
ethylbenzene	continental, water	3.49E-05	1.58E-08	1.34E-05	3.10E-11	1.34E-05	8.57E-14
ethylbenzene	continental, susp	3.47E-05	1.57E-08	1.33E-05	3.17E-11	1.33E-05	8.90E-14

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
ethylbenzene	continental, nat	1.73E-07	1.78E-05	1.23E-05	2.79E-12	1.23E-05	4.10E-14
ethylbenzene	continental, agr	1.25E-07	5.12E-05	2.09E-05	2.01E-12	2.09E-05	2.95E-14
ethylbenzene	continental, ind	1.73E-07	1.78E-05	1.23E-05	2.79E-12	1.23E-05	4.10E-14
ethylbenzene	north sea, air	8.60E-09	1.10E-08	9.10E-06	1.48E-11	9.10E-06	9.05E-12
ethylbenzene	north sea, seawater	1.21E-09	1.54E-09	1.29E-06	1.68E-09	1.29E-06	1.61E-09
ethylbenzene	north sea, seasusp	1.21E-09	1.54E-09	1.29E-06	1.67E-09	1.29E-06	1.61E-09
ethylbenzene	atlantic, air	8.62E-10	1.10E-09	7.59E-07	2.72E-11	7.59E-07	1.01E-14
ethylbenzene	atlantic, seawater	1.14E-10	1.46E-10	1.03E-07	1.70E-09	1.01E-07	9.23E-14
ethylbenzene	atlantic, seasusp	1.14E-10	1.46E-10	1.03E-07	1.70E-09	1.01E-07	1.26E-13
fluoranthene	regional, air	1.68E-01	3.47E-03	8.69E-02	9.89E-07	8.69E-02	1.62E-07
fluoranthene	regional, water	1.91E-01	4.81E-05	1.33E-03	1.79E-06	1.31E-03	6.13E-07
fluoranthene	regional, susp	1.75E-01	4.42E-05	1.22E-03	1.65E-06	1.21E-03	5.66E-07
fluoranthene	regional, nat	7.34E-02	4.63E-03	4.45E-03	6.60E-07	4.44E-03	2.18E-07
fluoranthene	regional, agr	4.08E-02	1.00E-02	1.41E+00	3.67E-07	1.41E+00	1.21E-07
fluoranthene	regional, ind	7.34E-02	4.63E-03	4.45E-03	6.60E-07	4.44E-03	2.18E-07
fluoranthene	continental, air	2.45E-01	4.46E-03	4.78E-02	5.75E-07	4.78E-02	2.89E-09
fluoranthene	continental, water	1.37E+00	3.20E-04	3.74E-03	1.47E-06	3.72E-03	3.35E-09
fluoranthene	continental, susp	1.37E+00	3.18E-04	3.72E-03	1.47E-06	3.70E-03	3.34E-09
fluoranthene	continental, nat	4.83E-01	4.77E-03	3.49E-03	5.33E-07	3.48E-03	1.29E-09
fluoranthene	continental, agr	2.68E-01	1.01E-02	1.35E-01	2.96E-07	1.35E-01	7.14E-10
fluoranthene	continental, ind	4.83E-01	4.77E-03	3.49E-03	5.33E-07	3.48E-03	1.29E-09
fluoranthene	north sea, air	1.17E-01	2.17E-03	2.73E-02	1.53E-06	2.73E-02	3.29E-07
fluoranthene	north sea, seawater	1.27E-03	2.35E-05	3.69E-04	3.08E-06	3.45E-04	1.06E-06
fluoranthene	north sea, seasusp	1.27E-03	2.35E-05	3.69E-04	3.08E-06	3.45E-04	1.06E-06
fluoranthene	atlantic, air	1.04E-02	1.90E-04	2.06E-03	2.38E-06	2.04E-03	2.60E-09
fluoranthene	atlantic, seawater	2.61E-04	4.75E-06	8.79E-05	3.12E-06	5.13E-05	3.07E-09
fluoranthene	atlantic, seasusp	2.61E-04	4.75E-06	8.79E-05	3.12E-06	5.13E-05	3.09E-09
fluorene	regional, air			2.40E-05	4.56E-10	2.40E-05	2.34E-10

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
fluorene	regional, water			7.12E-05	6.61E-09	7.12E-05	5.55E-09
fluorene	regional, susp			6.53E-05	6.21E-09	6.53E-05	5.22E-09
fluorene	regional, nat			2.25E-05	5.29E-10	2.25E-05	3.14E-10
fluorene	regional, agr			1.40E-02	4.28E-10	1.40E-02	2.53E-10
fluorene	regional, ind			2.25E-05	5.29E-10	2.25E-05	3.14E-10
fluorene	continental, air			1.08E-05	1.49E-10	1.08E-05	2.28E-12
fluorene	continental, water			1.88E-05	9.93E-10	1.88E-05	3.62E-12
fluorene	continental, susp			1.87E-05	1.01E-09	1.87E-05	3.69E-12
fluorene	continental, nat			9.86E-06	1.51E-10	9.86E-06	2.08E-12
fluorene	continental, agr			1.29E-03	1.22E-10	1.29E-03	1.68E-12
fluorene	continental, ind			9.86E-06	1.51E-10	9.86E-06	2.08E-12
fluorene	north sea, air			6.56E-06	8.98E-10	6.56E-06	5.35E-10
fluorene	north sea, seawater			4.12E-06	3.40E-08	4.08E-06	2.92E-08
fluorene	north sea, seasusp			4.12E-06	3.40E-08	4.08E-06	2.92E-08
fluorene	atlantic, air			4.74E-07	1.61E-09	4.59E-07	7.01E-13
fluorene	atlantic, seawater			5.47E-07	3.59E-08	2.23E-07	7.27E-12
fluorene	atlantic, seasusp			5.47E-07	3.59E-08	2.23E-07	7.88E-12
glycol	regional, air	1.13E-10			5.30E-14		5.07E-14
glycol	regional, water	1.37E-09			6.38E-13		6.09E-13
glycol	regional, susp	1.25E-09			5.91E-13		5.65E-13
glycol	regional, nat	4.82E-11			2.24E-14		2.15E-14
glycol	regional, agr	1.27E-11			5.93E-15		5.66E-15
glycol	regional, ind	4.82E-11			2.24E-14		2.15E-14
glycol	continental, air	1.87E-10			9.26E-15		2.26E-17
glycol	continental, water	2.26E-09			1.12E-13		2.69E-16
glycol	continental, susp	2.25E-09			1.12E-13		2.76E-16
glycol	continental, nat	7.95E-11			3.93E-15		9.48E-18
glycol	continental, agr	2.10E-11			1.04E-15		2.50E-18

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
glycol	continental, ind	7.95E-11			3.93E-15		9.48E-18
glycol	north sea, air	4.85E-15			1.45E-12		1.38E-12
glycol	north sea, seawater	6.66E-24			1.45E-12		1.38E-12
glycol	north sea, seasusp	6.66E-24			1.45E-12		1.38E-12
glycol	atlantic, air	1.71E-16			1.45E-12		9.67E-17
glycol	atlantic, seawater	2.21E-25			1.45E-12		9.67E-17
glycol	atlantic, seasusp	2.21E-25			1.45E-12		1.25E-16
lead	regional, air	5.82E-04	1.89E-06	7.06E-04	6.75E-07	7.06E-04	1.53E-08
lead	regional, water	2.18E-04		1.81E-05	1.27E-07	1.81E-05	1.02E-08
lead	regional, susp	2.00E-04		1.66E-05	1.24E-07	1.66E-05	9.97E-09
lead	regional, nat	1.09E-04	1.13E-06	9.03E-06	6.34E-08	9.03E-06	5.12E-09
lead	regional, agr	1.09E-04	4.52E-06	2.12E-02	6.34E-08	2.12E-02	5.12E-09
lead	regional, ind	1.09E-04	1.13E-06	9.03E-06	6.34E-08	9.03E-06	5.12E-09
lead	continental, air	7.58E-04	2.30E-06	1.98E-04	4.98E-07	1.98E-04	1.05E-09
lead	continental, water	1.88E-03		1.50E-05	2.11E-07	1.50E-05	3.32E-10
lead	continental, susp	1.87E-03		1.49E-05	2.10E-07	1.49E-05	3.32E-10
lead	continental, nat	9.42E-04	1.13E-06	7.49E-06	1.05E-07	7.49E-06	1.66E-10
lead	continental, agr	9.42E-04	4.52E-06	4.29E-04	1.05E-07	4.29E-04	1.66E-10
lead	continental, ind	9.42E-04	1.13E-06	7.49E-06	1.05E-07	7.49E-06	1.66E-10
lead	north sea, air	4.47E-04	1.37E-06	1.72E-04	9.07E-07	1.72E-04	3.05E-08
lead	north sea, seawater			1.87E-10	1.40E-06	5.20E-11	1.13E-07
lead	north sea, seasusp			1.87E-10	1.40E-06	5.19E-11	1.13E-07
lead	atlantic, air	5.63E-05	1.71E-07	1.48E-05	1.61E-06	1.48E-05	2.24E-09
lead	atlantic, seawater			1.78E-10	1.70E-06	1.06E-12	2.30E-09
lead	atlantic, seasusp			1.78E-10	1.70E-06	1.06E-12	2.31E-09
mercury	regional, air	9.83E-02	5.08E-04	1.07E-01	8.72E-05	1.07E-01	2.35E-06
mercury	regional, water	3.66E-02		8.46E-03	4.73E-05	8.46E-03	3.94E-06
mercury	regional, susp	3.35E-02		7.76E-03	4.58E-05	7.76E-03	3.81E-06

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
mercury	regional, nat	1.83E-02	3.04E-04	4.23E-03	2.36E-05	4.23E-03	1.97E-06
mercury	regional, agr	1.83E-02	1.22E-03	2.83E+00	2.36E-05	2.83E+00	1.97E-06
mercury	regional, ind	1.83E-02	3.04E-04	4.23E-03	2.36E-05	4.23E-03	1.97E-06
mercury	continental, air	1.28E-01	6.19E-04	3.65E-02	6.19E-05	3.65E-02	1.53E-07
mercury	continental, water	3.18E-01		7.05E-03	3.61E-05	7.05E-03	7.06E-08
mercury	continental, susp	3.17E-01		7.02E-03	3.60E-05	7.02E-03	7.04E-08
mercury	continental, nat	1.59E-01	3.04E-04	3.53E-03	1.80E-05	3.53E-03	3.53E-08
mercury	continental, agr	1.59E-01	1.22E-03	5.97E-02	1.80E-05	5.97E-02	3.53E-08
mercury	continental, ind	1.59E-01	3.04E-04	3.53E-03	1.80E-05	3.53E-03	3.53E-08
mercury	north sea, air	7.55E-02	3.68E-04	2.93E-02	1.18E-04	2.93E-02	4.57E-06
mercury	north sea, seawater			2.66E-07	2.04E-04	7.58E-08	1.70E-05
mercury	north sea, seasusp			2.66E-07	2.04E-04	7.57E-08	1.70E-05
mercury	atlantic, air	9.51E-03	4.60E-05	2.72E-03	1.84E-04	2.72E-03	2.82E-07
mercury	atlantic, seawater			1.98E-07	1.94E-04	1.28E-09	2.88E-07
mercury	atlantic, seasusp			1.98E-07	1.94E-04	1.29E-09	2.88E-07
methanol	regional, air			7.66E-06	9.36E-13	7.66E-06	1.97E-13
methanol	regional, water			1.52E-05	7.56E-13	1.52E-05	7.30E-13
methanol	regional, susp			1.39E-05	7.03E-13	1.39E-05	6.79E-13
methanol	regional, nat			3.38E-07	1.87E-14	3.38E-07	1.57E-14
methanol	regional, agr			1.70E-05	4.82E-15	1.70E-05	4.07E-15
methanol	regional, ind			3.38E-07	1.87E-14	3.38E-07	1.57E-14
methanol	continental, air			6.47E-06	7.50E-13	6.47E-06	7.98E-15
methanol	continental, water			2.07E-06	1.19E-13	2.07E-06	3.32E-16
methanol	continental, susp			2.06E-06	1.19E-13	2.06E-06	3.40E-16
methanol	continental, nat			6.37E-08	4.88E-15	6.37E-08	3.27E-17
methanol	continental, agr			2.68E-07	1.26E-15	2.68E-07	8.46E-18
methanol	continental, ind			6.37E-08	4.88E-15	6.37E-08	3.27E-17
methanol	north sea, air			4.37E-06	1.16E-12	4.37E-06	3.91E-13

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
methanol	north sea, seawater			2.70E-09	2.42E-12	2.70E-09	2.36E-12
methanol	north sea, seasusp			2.70E-09	2.42E-12	2.70E-09	2.36E-12
methanol	atlantic, air			6.23E-07	1.77E-12	6.23E-07	1.30E-15
methanol	atlantic, seawater			3.55E-10	2.42E-12	3.55E-10	9.50E-17
methanol	atlantic, seasusp			3.55E-10	2.42E-12	3.55E-10	1.44E-16
naphtalene	regional, air	9.31E-05	9.58E-07	3.29E-03	3.91E-10	3.29E-03	3.00E-10
naphtalene	regional, water	4.96E-02	5.07E-07	1.39E-01	5.69E-09	1.39E-01	5.32E-09
naphtalene	regional, susp	4.55E-02	4.65E-07	1.28E-01	5.31E-09	1.28E-01	4.96E-09
naphtalene	regional, nat	5.47E-03	1.41E-03	1.75E-02	9.05E-10	1.75E-02	7.98E-10
naphtalene	regional, agr	4.77E-03	4.92E-03	1.25E+01	7.89E-10	1.25E+01	6.96E-10
naphtalene	regional, ind	5.47E-03	1.41E-03	1.75E-02	9.05E-10	1.75E-02	7.98E-10
naphtalene	continental, air	1.34E-04	1.26E-06	9.53E-04	6.14E-11	9.53E-04	1.52E-12
naphtalene	continental, water	6.45E-02	8.51E-07	1.92E-02	8.06E-10	1.92E-02	2.56E-12
naphtalene	continental, susp	6.42E-02	8.47E-07	1.91E-02	8.13E-10	1.91E-02	2.62E-12
naphtalene	continental, nat	7.12E-03	1.41E-03	2.79E-03	1.33E-10	2.79E-03	1.40E-12
naphtalene	continental, agr	6.21E-03	4.92E-03	9.50E-01	1.16E-10	9.50E-01	1.22E-12
naphtalene	continental, ind	7.12E-03	1.41E-03	2.79E-03	1.33E-10	2.79E-03	1.40E-12
naphtalene	north sea, air	4.22E-05	4.02E-07	4.45E-04	9.87E-10	4.45E-04	8.01E-10
naphtalene	north sea, seawater	4.05E-06	3.86E-08	9.68E-05	2.14E-08	9.61E-05	2.02E-08
naphtalene	north sea, seasusp	4.05E-06	3.85E-08	9.68E-05	2.14E-08	9.60E-05	2.01E-08
naphtalene	atlantic, air	2.44E-06	2.30E-08	1.83E-05	1.41E-09	1.74E-05	3.35E-13
naphtalene	atlantic, seawater	2.26E-07	2.13E-09	1.48E-05	2.17E-08	1.62E-06	1.90E-12
naphtalene	atlantic, seasusp	2.26E-07	2.13E-09	1.48E-05	2.17E-08	1.62E-06	2.32E-12
nickel	regional, air	5.79E-05	4.64E-06	1.67E-03	1.80E-06	1.67E-03	3.96E-08
nickel	regional, water	2.05E-05		8.76E-04	2.39E-06	8.76E-04	1.99E-07
nickel	regional, susp	1.88E-05		8.05E-04	2.25E-06	8.05E-04	1.88E-07
nickel	regional, nat	1.02E-05	2.78E-06	4.38E-04	1.19E-06	4.38E-04	9.96E-08
nickel	regional, agr	1.02E-05	1.11E-05	4.24E-02	1.19E-06	4.24E-02	9.96E-08

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
nickel	regional, ind	1.02E-05	2.78E-06	4.38E-04	1.19E-06	4.38E-04	9.96E-08
nickel	continental, air	7.55E-05	5.66E-06	7.16E-04	1.53E-06	7.16E-04	3.41E-09
nickel	continental, water	1.88E-04		7.68E-04	2.06E-06	7.68E-04	3.83E-09
nickel	continental, susp	1.87E-04		7.64E-04	2.05E-06	7.64E-04	3.82E-09
nickel	continental, nat	9.38E-05	2.78E-06	3.84E-04	1.03E-06	3.84E-04	1.92E-09
nickel	continental, agr	9.38E-05	1.11E-05	1.23E-03	1.03E-06	1.23E-03	1.92E-09
nickel	continental, ind	9.38E-05	2.78E-06	3.84E-04	1.03E-06	3.84E-04	1.92E-09
nickel	north sea, air	4.45E-05	3.37E-06	5.33E-04	2.12E-06	5.33E-04	6.98E-08
nickel	north sea, seawater			3.62E-09	3.06E-06	1.03E-09	2.56E-07
nickel	north sea, seasusp			3.61E-09	3.06E-06	1.03E-09	2.56E-07
nickel	atlantic, air	5.60E-06	4.20E-07	5.33E-05	2.75E-06	5.33E-05	4.26E-09
nickel	atlantic, seawater			2.63E-09	2.85E-06	1.72E-11	4.27E-09
nickel	atlantic, seasusp			2.63E-09	2.85E-06	1.72E-11	4.27E-09
oil	regional, air		8.73E-15	1.17E-06	6.11E-14	1.17E-06	3.81E-16
oil	regional, water		2.61E-15	4.97E-07	6.07E-10	4.97E-07	5.86E-10
oil	regional, susp		2.40E-15	4.57E-07	5.87E-10	4.57E-07	5.66E-10
oil	regional, nat		1.91E-13	1.17E-06	6.11E-14	1.17E-06	4.09E-16
oil	regional, agr		7.38E-13	1.18E-06	6.11E-14	1.18E-06	4.09E-16
oil	regional, ind		1.91E-13	1.17E-06	6.11E-14	1.17E-06	4.09E-16
oil	continental, air		8.90E-15	1.14E-06	6.05E-14	1.14E-06	1.15E-16
oil	continental, water		5.81E-15	8.03E-07	2.05E-10	8.02E-07	5.08E-13
oil	continental, susp		5.78E-15	7.99E-07	2.07E-10	7.98E-07	5.17E-13
oil	continental, nat		1.91E-13	1.14E-06	6.05E-14	1.14E-06	1.15E-16
oil	continental, agr		7.38E-13	1.14E-06	6.05E-14	1.14E-06	1.15E-16
oil	continental, ind		1.91E-13	1.14E-06	6.05E-14	1.14E-06	1.15E-16
oil	north sea, air		8.51E-15	1.10E-06	6.19E-14	1.10E-06	6.49E-16
oil	north sea, seawater		1.20E-15	2.70E-07	7.03E-09	2.69E-07	6.78E-09
oil	north sea, seasusp		1.20E-15	2.70E-07	7.03E-09	2.69E-07	6.78E-09

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	**Emission region, compartment**	**Aquatic ecotoxicity**	**Terrestrial ecotoxicity**	**Human toxicity**	**Marine ecotoxicity**	**Human toxicity**	**Marine ecotoxicity**
oil	atlantic, air		7.33E-15	9.41E-07	6.64E-14	9.41E-07	1.01E-16
oil	atlantic, seawater		9.59E-16	1.50E-07	7.17E-09	1.23E-07	4.04E-13
oil	atlantic, seasusp		9.59E-16	1.50E-07	7.17E-09	1.23E-07	5.44E-13
phenantrene	regional, air	2.56E-05	2.06E-06	2.94E-04	7.09E-09	2.94E-04	4.21E-09
phenantrene	regional, water	1.07E-02	1.07E-06	5.45E-04	1.89E-07	5.45E-04	1.29E-07
phenantrene	regional, susp	9.83E-03	9.80E-07	5.00E-04	1.75E-07	4.99E-04	1.20E-07
phenantrene	regional, nat	1.60E-03	6.40E-04	2.09E-04	3.11E-08	2.08E-04	2.10E-08
phenantrene	regional, agr	8.90E-04	1.43E-03	2.68E-01	1.73E-08	2.68E-01	1.17E-08
phenantrene	regional, ind	1.60E-03	6.40E-04	2.09E-04	3.11E-08	2.08E-04	2.10E-08
phenantrene	continental, air	4.18E-05	2.70E-06	7.07E-05	8.86E-10	7.07E-05	1.68E-11
phenantrene	continental, water	1.89E-02	2.27E-06	1.50E-04	3.69E-08	1.50E-04	9.21E-11
phenantrene	continental, susp	1.88E-02	2.26E-06	1.49E-04	3.69E-08	1.49E-04	9.33E-11
phenantrene	continental, nat	2.81E-03	6.41E-04	5.32E-05	5.84E-09	5.32E-05	2.10E-11
phenantrene	continental, agr	1.57E-03	1.43E-03	2.50E-02	3.26E-09	2.50E-02	1.17E-11
phenantrene	continental, ind	2.81E-03	6.41E-04	5.32E-05	5.84E-09	5.32E-05	2.10E-11
phenantrene	north sea, air	1.04E-05	6.88E-07	2.89E-05	2.01E-08	2.89E-05	1.24E-08
phenantrene	north sea, seawater	2.97E-06	1.96E-07	1.93E-05	4.37E-07	1.82E-05	3.00E-07
phenantrene	north sea, seasusp	2.96E-06	1.96E-07	1.93E-05	4.37E-07	1.82E-05	3.00E-07
phenantrene	atlantic, air	5.42E-07	3.50E-08	1.13E-06	2.71E-08	9.19E-07	1.46E-11
phenantrene	atlantic, seawater	2.05E-07	1.33E-08	3.86E-06	4.52E-07	3.57E-07	2.08E-10
phenantrene	atlantic, seasusp	2.05E-07	1.33E-08	3.86E-06	4.52E-07	3.57E-07	2.14E-10
phenol	regional, air	3.14E-05	6.40E-07	2.14E-06	1.19E-11	2.14E-06	1.01E-11
phenol	regional, water	1.48E-02	4.24E-08	6.94E-06	9.39E-11	6.94E-06	9.27E-11
phenol	regional, susp	1.36E-02	3.89E-08	6.36E-06	8.86E-11	6.36E-06	8.74E-11
phenol	regional, nat	2.64E-03	6.95E-04	1.60E-06	1.88E-11	1.60E-06	1.83E-11
phenol	regional, agr	1.10E-03	1.15E-03	2.06E-04	7.79E-12	2.06E-04	7.57E-12
phenol	regional, ind	2.64E-03	6.95E-04	1.60E-06	1.88E-11	1.60E-06	1.83E-11
phenol	continental, air	4.41E-05	8.42E-07	5.43E-07	1.47E-12	5.43E-07	4.24E-14

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
phenol	continental, water	1.73E-02	6.52E-08	8.14E-07	1.17E-11	8.14E-07	2.43E-14
phenol	continental, susp	1.72E-02	6.49E-08	8.10E-07	1.19E-11	8.10E-07	2.56E-14
phenol	continental, nat	3.10E-03	6.95E-04	2.39E-07	2.34E-12	2.39E-07	1.16E-14
phenol	continental, agr	1.28E-03	1.15E-03	3.95E-06	9.69E-13	3.95E-06	4.81E-15
phenol	continental, ind	3.10E-03	6.95E-04	2.39E-07	2.34E-12	2.39E-07	1.16E-14
phenol	north sea, air	1.17E-05	2.25E-07	2.23E-07	3.29E-11	2.23E-07	2.91E-11
phenol	north sea, seawater	4.75E-08	9.13E-10	9.22E-10	5.70E-10	9.22E-10	5.63E-10
phenol	north sea, seasusp	4.74E-08	9.13E-10	9.21E-10	5.69E-10	9.21E-10	5.62E-10
phenol	atlantic, air	6.08E-07	1.16E-08	7.49E-09	4.38E-11	7.49E-09	6.48E-15
phenol	atlantic, seawater	2.25E-09	4.30E-11	3.09E-11	5.70E-10	2.78E-11	1.05E-14
phenol	atlantic, seasusp	2.26E-09	4.30E-11	3.10E-11	5.70E-10	2.78E-11	2.21E-14
toluene	regional, air	1.10E-08	2.88E-08	9.24E-06	3.25E-11	9.24E-06	1.41E-11
toluene	regional, water	1.73E-05	2.20E-08	1.76E-05	7.12E-10	1.76E-05	6.55E-10
toluene	regional, susp	1.58E-05	2.02E-08	1.61E-05	6.72E-10	1.61E-05	6.19E-10
toluene	regional, nat	1.14E-07	2.35E-05	8.44E-06	3.36E-11	8.44E-06	1.67E-11
toluene	regional, agr	9.08E-08	7.48E-05	7.93E-05	2.67E-11	7.93E-05	1.33E-11
toluene	regional, ind	1.14E-07	2.35E-05	8.44E-06	3.36E-11	8.44E-06	1.67E-11
toluene	continental, air	1.37E-08	3.53E-08	4.98E-06	1.45E-11	4.98E-06	1.92E-13
toluene	continental, water	2.00E-05	3.02E-08	5.58E-06	9.94E-11	5.58E-06	3.16E-13
toluene	continental, susp	1.99E-05	3.01E-08	5.55E-06	1.01E-10	5.55E-06	3.25E-13
toluene	continental, nat	1.34E-07	2.36E-05	4.53E-06	1.36E-11	4.53E-06	1.75E-13
toluene	continental, agr	1.06E-07	7.48E-05	7.43E-06	1.08E-11	7.43E-06	1.39E-13
toluene	continental, ind	1.34E-07	2.36E-05	4.53E-06	1.36E-11	4.53E-06	1.75E-13
toluene	north sea, air	7.75E-09	2.00E-08	3.31E-06	5.69E-11	3.31E-06	3.08E-11
toluene	north sea, seawater	1.84E-09	4.75E-09	7.90E-07	4.45E-09	7.90E-07	4.16E-09
toluene	north sea, seasusp	1.84E-09	4.75E-09	7.89E-07	4.44E-09	7.89E-07	4.16E-09
toluene	atlantic, air	8.72E-10	2.24E-09	3.17E-07	1.08E-10	3.17E-07	4.67E-14
toluene	atlantic, seawater	2.02E-10	5.21E-10	7.46E-08	4.57E-09	7.36E-08	4.26E-13

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	**Emission region, compartment**	**Aquatic ecotoxicity**	**Terrestrial ecotoxicity**	**Human toxicity**	**Marine ecotoxicity**	**Human toxicity**	**Marine ecotoxicity**
toluene	atlantic, seasusp	2.02E-10	5.21E-10	7.46E-08	4.57E-09	7.36E-08	5.12E-13
xylene	regional, air	1.00E-08	1.32E-08	2.29E-06	3.44E-11	2.29E-06	2.32E-11
xylene	regional, water	3.71E-05	1.03E-08	2.88E-06	1.86E-09	2.88E-06	1.71E-09
xylene	regional, susp	3.40E-05	9.46E-09	2.64E-06	1.75E-09	2.64E-06	1.61E-09
xylene	regional, nat	2.49E-07	2.52E-05	2.12E-06	4.36E-11	2.12E-06	3.24E-11
xylene	regional, agr	2.06E-07	8.35E-05	1.31E-05	3.62E-11	1.31E-05	2.69E-11
xylene	regional, ind	2.49E-07	2.52E-05	2.12E-06	4.36E-11	2.12E-06	3.24E-11
xylene	continental, air	1.35E-08	1.71E-08	8.07E-07	7.42E-12	8.07E-07	1.54E-13
xylene	continental, water	4.33E-05	1.51E-08	8.57E-07	2.40E-10	8.57E-07	5.42E-13
xylene	continental, susp	4.30E-05	1.51E-08	8.52E-07	2.45E-10	8.52E-07	5.66E-13
xylene	continental, nat	2.92E-07	2.52E-05	7.47E-07	8.37E-12	7.47E-07	1.45E-13
xylene	continental, agr	2.42E-07	8.35E-05	1.36E-06	6.94E-12	1.36E-06	1.20E-13
xylene	continental, ind	2.92E-07	2.52E-05	7.47E-07	8.37E-12	7.47E-07	1.45E-13
xylene	north sea, air	5.35E-09	6.80E-09	4.33E-07	7.81E-11	4.33E-07	5.75E-11
xylene	north sea, seawater	1.54E-09	1.96E-09	1.26E-07	1.15E-08	1.26E-07	1.06E-08
xylene	north sea, seasusp	1.54E-09	1.96E-09	1.26E-07	1.15E-08	1.26E-07	1.06E-08
xylene	atlantic, air	3.66E-10	4.63E-10	2.19E-08	1.25E-10	2.19E-08	3.77E-14
xylene	atlantic, seawater	1.06E-10	1.34E-10	6.55E-09	1.18E-08	6.32E-09	1.33E-12
xylene	atlantic, seasusp	1.06E-10	1.34E-10	6.55E-09	1.18E-08	6.32E-09	1.55E-12
zinc	regional, air	1.41E-04	1.16E-06	3.99E-03	1.97E-07	3.99E-03	5.00E-09
zinc	regional, water	5.24E-05		1.24E-05	9.94E-08	1.24E-05	8.23E-09
zinc	regional, susp	4.80E-05		1.14E-05	9.44E-08	1.14E-05	7.82E-09
zinc	regional, nat	2.62E-05	6.95E-07	6.19E-06	4.97E-08	6.19E-06	4.12E-09
zinc	regional, agr	2.62E-05	2.78E-06	2.83E-03	4.97E-08	2.83E-03	4.12E-09
zinc	regional, ind	2.62E-05	6.95E-07	6.19E-06	4.97E-08	6.19E-06	4.12E-09
zinc	continental, air	1.84E-04	1.42E-06	2.85E-03	1.45E-07	2.85E-03	3.39E-10
zinc	continental, water	4.57E-04		1.04E-05	9.80E-08	1.04E-05	1.76E-10
zinc	continental, susp	4.55E-04		1.03E-05	9.77E-08	1.03E-05	1.75E-10

		general		*include all exposure routes*		*exclude exposure via ocean*	
Substance	Emission region, compartment	Aquatic ecotoxicity	Terrestrial ecotoxicity	Human toxicity	Marine ecotoxicity	Human toxicity	Marine ecotoxicity
zinc	continental, nat	2.29E-04	6.95E-07	5.18E-06	4.90E-08	5.18E-06	8.78E-11
zinc	continental, agr	2.29E-04	2.78E-06	6.14E-05	4.90E-08	6.14E-05	8.78E-11
zinc	continental, ind	2.29E-04	6.95E-07	5.18E-06	4.90E-08	5.18E-06	8.78E-11
zinc	north sea, air	1.08E-04	8.41E-07	1.86E-03	2.63E-07	1.86E-03	9.72E-09
zinc	north sea, seawater			2.84E-12	4.35E-07	8.05E-13	3.61E-08
zinc	north sea, seasusp			2.84E-12	4.35E-07	8.04E-13	3.60E-08
zinc	atlantic, air	1.37E-05	1.05E-07	2.12E-04	4.12E-07	2.12E-04	6.19E-10
zinc	atlantic, seawater			2.21E-12	4.33E-07	1.41E-14	6.32E-10
zinc	atlantic, seasusp			2.21E-12	4.33E-07	1.41E-14	6.32E-10

Appendix B TOXICITY DATA

Reported EC50 figure represents the geometric mean in those cases where number > 1

Test species	EC50	StDev	number
Toluene			
Artemia salina	13950	19165	2
Branchionus calyciflorus	113		1
Branchionus plicatilis	553		1
Cancer magister	28000		1
Carassius auratus	57680	0	6
Crago franciscorum	6228	4721	2
Crangon franciscorum	4300		1
Crassostrea gigas	172000		1
Daphnia magna	1150		1
Eualus sp	18522	3573	3
Hemigrapsus nudus	24613	2021	3
Lebistes reticulates	61003	1756	3
Lepomis macrochirus	31707	10943	6
Morone saxatilis	6961	501	6
Oncorhynchus gorbuscha	7097	858	4
Oncorhynchus kisutch	40763	114839	7
Palaemonetes pugio	9600		1
Pimephales promelas	46225	7940	12
Poecilia reticulata	61003	1756	3
Selenastrum capricornutum	9400	NA	1
Benzene			
Aedes aegypti	200000		1
Ambystoma mexicanum	370000		1
Artemia salina	16340	5859.	2
Asellus aquaticus	120000		1
Cancer magister	108000		1
Carassius auratus	34420	0	6
Chironimus sp	100000		1
Cloeon dipterum	34000		1
Clupea harengus pallasi	28926	11236	5
Corixa punctata	48000		1
Cottus cognatus	13799	1248	2
Crago franciscorum	18438	1243	2
Crassostrea gigas	377000		1
Culex pipiens	71000		1
Cyprinodon variegatus	22900		1
Daphnia cucculata	373000		1
Daphnia magna	35327	280636	2
Daphnia pulex	305000		1
Dugesia sp	74000		1
Eleginis gracilis	9046	2817	6
Engraulis mordax	22407	2500	3

Test species	EC50	StDev	number
Gammarus pulex	42000		1
Gasterosteus aculeatus	14456	1307	2
Hydra oligactis	34000	0	2
Ischnura elegans	10000		1
Lebistes reticulates	36600	0	3
Lepomis macrochirus	22490	0	6
Leuciscus idus	132000		1
Lymnaea stagnalis	230000	0	2
Morone saxatilis	7110	2319	6
Nemoura cinerea	130000		1
Oncorhynchus gorbuscha	11245	4805	4
Oncorhynchus kisutch	17192	18992	4
Oncorhynchus nerka	6355	2476	3
Oncorhynchus tshawytscha	34797	64696	2
Oryzias latipes	250000		1
Palaemonetes pugio	27000		1
Palaemonetes sp	29258	5773	3
Penaeus monodon	23292	2107	2
Pimephales promelas	36247	13994	13
Poecilia reticulata	42000		1
Salmo gairdneri	17228	35850	2
Selenastrum capricornutum	41000		1
Xenopus laevis	190000		1
Ethylbenzene			
Carassius auratus	94440	0	6
Crago franciscorum	900	1048	2
Daphnia magna	2100		1
Lebistes reticulates	97100	0	3
Lepomis macrochirus	33996	1570	6
Morone saxatilis	4004	330	4
Mysidopsis bahia	88000		1
Oncorhynchus kisutch	22361	28284	2
Palaemonetes pugio	11832	2828	2
Pimephales promelas	45315	3227	12
Poecilia reticulata	97100	0	3
Selenastrum capricornutum	4800		1
Xylene			
Artemia salina	2227	246	4
Branchionus calyciflorus	253		1
Branchionus plicatilis	496		1
Cancer magister	6000		1
Carassius auratus	33821	8452	9
Crago franciscorum	2438	1450	6
Crangon franciscorum	1300		1
Crassostrea gigas	11000		1
Cyprinus carpio	16000		1
Daphnia magna	618	331	3

Test species	EC50	StDev	number
Gambusia affinis	24000	0	2
Lebistes reticulates	34730	0	3
Lepomis macrochirus	4917	9770	10
Morone saxatilis	5064	3936	13
Oncorhynchus kisutch	31623	63640	2
Palaemonetes pugio	7400		1
Photobacterium phosphoreum	1600		1
Pimephales promelas	25869	4793	14
Poecilia reticulata	34730	0	4
Rutilus rutilus	21000	0	2
Salmo gairdneri	5292	2121	2
Selenastrum capricornutum	4162	252	3
Strongylocentrotus droebachiensis	4100		1
Fluoranthene			
Nereis arenaceodentata	500		1
Naphthalene			
Artemia salina	1497	741	2
Cyprinodon variegatus	2400		1
Daphnia magna	472		1
Daphnia pulex	3394	8	2
Elasmopus pectinicrus	2927	468	4
Eurytemora affinis	3800		1
Hemigrapsus nudus	1502	981	3
Neomysis americana	850		1
Nereis arenaceodentata	3800		1
Oncorhynchus gorbuscha	696	336	7
Oncorhynchus kisutch	5180	3784	5
Palaemonetes pugio	2350	0	2
Palaemonetes sp	2300	0	2
Pandalus goniurus	1289	673	3
Penaeus aztecus	2500	0	2
Pimephales promelas	6400	1061	2
Salmo gairdneri	1600		1
Phenol			
Agonus cataphractus	10000		1
Artemia salina	56000		1
Carassius auratus	47766	2605	6
Crangon crangon	19000		1
Crangon septemspinosa	7500		1
Crassostrea gigas	58250		1
Gammarus duebeni	32500		1
Kuhlia sandvicensis	11000		1
Lebistes reticulates	46014	6160	3
Lepomis macrochirus	24506	1028	6
Mercenaria mercenaria	52630		1
Mesidotea entomon	85800		1

Test species	EC50	StDev	number
Mugil saliens	15500		1
Mya arenaria	441899	120208	2
Ophryotrocha diadema	215000		1
Palaemonetes pugio	5800		1
Palaemonetes sp	17145	18148	3
Paralichtys olivaceus	300		1
Phoxinus phoxinus	9500		1
Pimephales promelas	37596	3373	11
Platichthys flesus	66500		1
Poecilia reticulata	46014	6160	3
Pseudopleuronectes yokohamae	100		1
Stolephorus purpureus	510		1
Phenanthrene			
Daphnia pulex	1140		1
Nereis arenaceodentata	600		1
Fluorene			
TestSpecies	EC50	StDev	total
Carassius auratus	5000		1
Pimephales promelas	100000		1
Daphnia magna	430		1
Lepomis macrochirus	3100		1
Neanthes arenaceodentata	1000		1
Biphenyl			
Daphnia magna	684	665	2
Methanol			
Artemia salina	10000000		1
Salmo gairdneri	8000000		1
Nickel			
Allorchestes compressa	12280		1
Artemia salina	4660		1
Cancer magister	4360		1
Chelon labrosus	118300		1
Crangon crangon	210000		1
Crassostrea gigas	349		1
Crassostrea virginica	30		1
Ctenodrilus serratus	7700		1
Gymnodinium splendens	3500		1
Mercenaria mercenaria	310		1
Morone saxatilis	21000		1
Mysidopsis bahia	508		1
Mytilus edulis	891		1
Nereis arenaceodentata	7700		1
Nitocra spinipes	6000		1
Thalassiosira guillardii	100		1

Test species	EC50	StDev	number
Thalassiosira rotula	300		1
Therapon jarbua	19400		1
Chromium			
Agonus cataphractus	66500		1
Amphipod (SG) none	19270		1
Capitella capitata	280		1
Cerastoderma edule	215000		1
Crangon crangon	100000		1
Crassostrea rhizophorae	7000		1
Crassostrea virginica	10300		1
Ctenodrilus serratus	4300		1
Ditylum brightwelli	2000		1
Gymnodinium splendens	220		1
Nereis arenaceodentata	550		1
Ophiothrix spiculata	1700		1
Ophryotrocha diadema	100000		1
Palaemonetes pugio	4860		1
Thalassiosira guillardii	350		1
Lead			
Argopecten irradians	8600		1
Artemia salina	85		1
Cancer magister	575		1
Capitella capitata	1000		1
Ceriodaphnia reticulata	1878		1
Chlorella stigmatophora	700		1
Crangon crangon	20		1
Crassostrea gigas	758		1
Crassostrea virginica	2450		1
Ctenodrilus serratus	1900		1
Daphnia magna	269	830	5
Daphnia pulex	2003		1
Dicentrarchus labrax	65		1
Ditylum brightwelli	40		1
Enoplus brevis	10		1
Enoplus communis	10		1
Menidia beryllina	13500		1
Mercenaria mercenaria	780		1
Mysidopsis bahia	3130		1
Mytilus edulis	100		1
Nereis arenaceodentata	1040		1
Ophryotrocha diadema	1700		1
Ophryotrocha labronica	1000		1
Perna viridis	2450		1
Pleuronectes platessa	39		1
Spisula solidissima	5400		1
Therapon jarbua	1230		1
Uronema marinum	60000		1

Test species	EC50	StDev	number
Mercury			
Allorchestes compressa	80		1
Anadara broughtoni	4840		1
Argopecten irradians	89		1
Balanus balanoides	90		1
Balanus crenatus	60		1
Cancer magister	8.2		1
Capitella capitata	14		1
Carcinus maenas	14		1
Cerastoderma edule	9600		1
Crangon crangon	10		1
Crassostrea gigas	6.7		1
Crassostrea virginica	5.6		1
Crepidula fornicata	60		1
Ctenodrilus serratus	90		1
Dinophilus gyrociliatus	100		1
Ditylum brightwelli	10		1
Enoplus brevis	10		1
Enoplus communis	10		1
Fundulus heteroclitus	37.2		1
Gammarus duebeni	122		1
Gymnodinium splendens	15		1
Homarus americanus	20		1
Homarus gammarus	66.5		1
Isochrysis galbana	90		1
Mercenaria mercenaria	4.8		1
Meretrix lusoria	670		1
Mysidopsis bahia	1.8		1
Mytilus edulis	5.8		1
Nereis arenaceodentata	17		1
Nitocra spinipes	230		1
Ophryotrocha diadema	90		1
Oplegnathus fasciatus	1400		1
Ostrea edulis	17		1
Palaemonetes pugio	38		1
Palaemonetes vulgaris	7.4		1
Paralichtys olivaceus	50		1
Penaeus indicus	15.3		1
Penaeus setiferus	17		1
Petrolisthes armatus	50		1
Platichthys flesus	3300		1
Pseudopleuronectes yokohamae	300		1
Rangia cuneata	57		1
Scylla serrata	540		1
Seriola quinqueradiata	110		1
Skeletonema costatum	13		1
Thalassiosira guillardii	30		1
Therapon jarbua	60		1

Test species	EC50	StDev	number
Uronema marinum	6		1
Zinc			
Abramis brama	14300		1
Acartia lilljeborgi	633	206	5
Acartia simplex	1860		1
Acartia spinicauda	390		1
Achnanthes lanceolata	4144	2421	3
Achnanthes linearis	15363	34174	2
Achnanthes minutissima	30144	30983	8
Agosia chrysogaster	790		1
Alburnus alburnus	36617	7000	2
Aldrichetta forsteri	12750		1
Allorchestes compressa	1077	1004	2
Ancylus fluviatilis	388	1190	18
Anguilla anguilla	63000		1
Anguilla rostrata	18476	3668	3
Aphanocapsa montana	2120		1
Arenicola marina	136		1
Argopecten irradians	2250		1
Artemia fransiscana	65		1
Artemia salina	1761	1485	2
Asellus aquaticus	26400		1
Asellus intermedius	1300		1
Aspidisca cicada	2400		1
Asterias forbesi	32705	214032	3
Atherinasoma microstoma	37000		1
Blephiarisma americanum	1050		1
Brachionus calyciflorus	1300		1
Bufo melanostictus	33128	15176	4
Bugula neritina	5000		1
Callianassa australiensis	2446	4335	4
Cancer magister	517	92	2
Capitella capitata	2077	988	4
Carassius auratus	7643	1860	2
Carcinus maenas	6619	9777	3
Cardia edule	200000		1
Cerastoderma edule	215000		1
Chaetophoraceae pseudendoclonium	12707	20280	2
Chamaesiphon polymorphus	270		1
Channa punctatus	34647	17236	25
Characium angustum	14800		1
Charybdis feriatus	960		1
Chelon labrosus	26135	8617	3
Chironomus tentans	110	49	2
Chlorella saccharophila	46900		1
Chlorococcum sp	13000		1
Chlorolobion braunii	21700		1
Colpidium campylum	1850		1

Test species	EC50	StDev	number
Corbicula fluminea	1910	3844	2
Corophium volutator	10954	34324	44
Cosmarium sublateriundatum	14030	1980	2
Crangon crangon	10084	46680	4
Crassostrea cucculata	82	40	3
Crassostrea gigas	63	406	5
Crassostrea margaritacea	77	31	4
Crassostrea rhizophorae	16000		1
Crassostrea virginica	610	629	2
Ctenodrilus serratus	1770		1
Cyclops abyssorum	5500		1
Cymbella minuta	15400		1
Cyprinus carpio	10123	3403	3
Daphnia hyalina	40		1
Daphnia magna	456	6242	19
Ditylum brightwelli	100		1
Draparnaldia plumosa	5110		1
Dugesia tigrina	13000		1
Enoplus brevis	10		1
Enoplus communis	10		1
Ephemerella subvaria	16000		1
Erpobdella octoculata	1027	4581	3
Eudiaptomus padanus	500		1
Eunotia pectinalis	4070		1
Euplotes affinis	3100		1
Euplotes palella	50000		1
Fragilaria vaucheriae	15800		1
Fundulus diaphanus	20751	1752	3
Fundulus heteroclitus	73061	40037	3
Gammarus fasciatus	4050		1
Gammarus pulex	4130	2080	5
Gomphonema angustatum	3330		1
Gomphonema gracile	4670		1
Gomphonema parvulum	2956	1090	3
Gymnodinium splendens	1500		1
Haliotis rufescens	58	13	2
Helisoma trivolvis	13000		1
Holmesimysis costata	211	255	2
Isochrysis galbana	800		1
Jordanella floridae	1500		1
Klebsormidium klebsii	11800		1
Lebistes reticulates	6899	57655	18
Lemna minor	10000		1
Lepomis gibbosus	22231	2641	3
Lepomis macrochirus	6202	1957	14
Lumbriculus variegatus	1300		1
Lymnaea emerginata	4150		1
Lymnaea luteola	6961	5079	20
Macoma balthica	422	562	27

Test species	EC50	StDev	number
Melosira varians	6670		1
Mercenaria mercenaria	180	21	2
Microthamnion kuetzingianum	9680		1
Moina marocopa	269	810	9
Monhystera disjuncta	1900	16051	2
Morone saxatilis	430		1
Mya arenaria	8011	110705	8
Mysidopsis bahia	498	1	2
Mysidopsis juniae	363		1
Mytilus edulis	4579	7897	5
Myxosarcina burmensis	1910		1
Nassarius obsoletus	38144	73200	3
Navicula secura	5660		1
Neanthes arenaceodentata	1252	395	9
Neanthes vaali	5500		1
Neidium bisulcatum	2290		1
Nereis arenaceodentata	720		1
Nereis diversicolor	27679	148238	10
Nereis grubei	1800		1
Nereis virens	7496	8894	3
Nitocra spinipes	233	1458	9
Nitzschia clasterium	320	64	2
Nitzschia communis	32000		1
Nitzschia ignorata	2220		1
Nitzschia linearis	5730		1
Noemacheilus barbatulus	2500		1
Oncorhynchus tshawytscha	3996	5005	4
Oocystis borgei	38300		1
Oocystis lacustris	58437	32527	2
Ophryotrocha diadema	330		1
Ophryotrocha labronica	1342	566	2
Orconectes virilis	84000		1
Pagurus longicarpus	986	6756	3
Palaemon serratus	12806	40133	3
Palaemon sp	9500		1
Palaemonetes varians	38400		1
Pandalus montagui	10000		1
Paracalanus parvus	1380		1
Paragrapsus quadridentatus	6287	4807	4
Paramecium caudatum	2500		1
Paratya compressa	800		1
Paratya tasmaniensis	1210		1
Parophrys vetulus	14500		1
Pectinaria californiensis	2800		1
Penaeus merguiensis	882	1888	5
Perca fluviatilus	16000		1
Perna viridis	2635	2525	3
Phaeodactylum tricornutum	270		1
Phormidium foveolarum	506	247	2

Test species	EC50	StDev	number
Phormidium jenkelianum	1152	1478	2
Phormidium molle	467	629	2
Phormidium mucicola	765	127	2
Phormidium ramosum	3215	566	2
Phormidium sp	1190	1648	2
Phormidium uncinatum	930		1
Phoxinus phoxinus	3200		1
Physa gyrina	4400		1
Pimephales promelas	4290	11192	22
Pinnularia brevicostata	9410		1
Pinnularia burkii	6150		1
Pinnularia substomatophora	4280		1
Pinnularia viridis	8430		1
Plectonema radiosum	210		1
Poecilia reticulata	2962	2319	4
Portunus pelagicus	560		1
Portunus sanguinolentus	620		1
Puntius sophore	42509	27244	18
Rasbora Daniconius	40411	9356	5
Roccus americanus	12565	2193	3
Roccus saxatilis	9087	2330	3
Rutilus rutilus	17300		1
Salmo gairdneri	1271	7136	33
Salmo irideus	4000		1
Salmo salar	768	610	6
Scenedesmus acutus	77367	20011	2
Scrobicularia plana	10000		1
Scutellidium sp	1090		1
Scyliorhinus canicula	80000		1
Scylla serrata	161200		1
Spirorbis lamellosa	5000		1
Spisula solidissima	2950		1
Stichococcus bacillaris	51700		1
Stigeoclonium aestivale	13600		1
Stigeoclonium fasciculare	20500		1
Stigeoclonium sp	16800		1
Surirella augustata	13900		1
Surirella ovata	3260		1
Synedra acus	7580		1
Synedra rumpens	6046	4118	4
Synedra sp	13300		1
Synedra ulna	6630	5049	2
Tanytarsus dissimilis	37		1
Temora stylifera	17	13	4
Thalassiosira guillardii	500	0	2
Therapon jarbua	11992	5048	5
Tigriopus brevicornis	325		1
Tisbe holothuriae	721	300	4
Tortanus forcipatus	750		1

Test species	EC50	StDev	number
Tubifex tubifex	3012	24554	13
Ulothrix zonata	4113	10946	3
Uronema gigas	45900		1
Uronema marinum	362792	178401	3
Uronema nigricans	2900		1
Viviparus Bengalensis	7894	7761	5
Vorticella convallaria	290		1
Watersipora calcullata	33000		1
Copper			
Acartia simplex	200	0	2
Acartia spinicauda	10	0	2
Acartia tonsa	23	20	4
Agonus cataphractus	60		1
Allorchestes compressa	124	230	5
Amphiura filiformis	615	1896	11
Anadara broughtoni	310		1
Anadara granosa	60	0	2
Archosargus probatocephalus	1140		1
Arenicola marina	13685	14323	10
Argopecten irradians	6	28	8
Arius felis	2400		1
Artemia salina	485		1
Asellus aquaticus	308	3398	9
Balanus balanoides	1455	1064	5
Balanus improvisus	88		1
Branchionus plicatilis	125	7	2
Callianassa australiensis	294	330	6
Cancer magister	49	0	2
Capitella capitata	160	50	5
Carcinus maenas	932	3826	6
Cardia edule	3162	6364	2
Cerastoderma edule	1000		1
Cerethidea cingulata	12500		1
Chelon labrosus	1424	50	4
Chlorella stigmatophora	70		1
Choromytilus meridionalis	214	21	2
Clupea harengus	338	1276	9
Clupea harengus pallasi	33		1
Crangon crangon	2086	27916	13
Crassostrea gigas	61	621	5
Crassostrea madrasensis	88	0	2
Crassostrea margaritacea	65	214	7
Crassostrea rhizophorae	2500		1
Crassostrea virginica	33		1
Ctenodrilus serratus	300		1
Daphnia magna	20	27	6
Ditylum brightwelii	15		1
Echinometra mathaei	341	100	4

Test species	EC50	StDev	number
Engraulis mordax	185		1
Enoplus brevis	158	4367	5
Enoplus communis	10		1
Fucus serratus	143	192	4
Fucus spiralis	171	155	6
Fucus vesiculosus	219	320	7
Fundulus heteroclitus	1000		1
Haliotis cracherodii	50		1
Haliotis rufescens	65		1
Homarus americanus	243	340	20
Homarus gammarus	5	173	3
Lagodon rhomboides	2750		1
Leiostomus xanthurus	6400		1
Limanda limanda	389	91	3
Macoma balthica	403	468	6
Menidia menidia	1300		1
Mercenaria mercenaria	16		1
Meretrix casta	203	288	4
Meretrix lusoria	7040		1
Micropogonias undulatus	5660		1
Monhystera disjuncta	2400		1
Morone saxatilis	190		1
Mya arenaria	124	2482	4
Mysidopsis almyra	181		1
Mytilus edulis	6	1035	22
Neanthes arenaceodentata	210	84	5
Nereis arenaceodentata	140		1
Nereis diversicolor	299	173	4
Nereis grubei	100		1
Nitocra spinipes	1800		1
Nitzschia closterium	32		1
Ophryotrocha diadema	179	28	2
Ophryotrocha labronica	166	414	5
Oplegnathus fasciatus	1730		1
Palaemonetes pugio	12800		1
Pandalus danae	21		1
Paracalanus parvus	190	0	2
Paracentrotus lividus	37	11	4
Paragrapsus quadridentatus	137	42	2
Pecten maximus	85		1
Pelvetia canaliculata	143	154	7
Penaeus merguiensis	581	2143	7
Perna perna	224	35	2
Perna viridis	55	347	3
Phaeodactylum tricornutum	33		1
Pimephales promelas	2		1
Platichthys flesus	2250		1
Polinices incei	1170	57	2
Rangia cuneata	2269	6022	12

Test species	EC50	StDev	number
Scrobicularia plana	240		1
Scutellidium sp	180		1
Scyliorhinus canicula	4000		1
Scylla serrata	137800		1
Seriola quinqueradiata	1030		1
Skeletonema costatum	5		1
Spisula solidissima	23	29	2
Thalassiosira guillardii	3		1
Therapon jarbua	5834	2170	5
Tisbe holothuriae	255	177	7
Tortanus forcipatus	40	0	2
Trachinotus carolinus	560		1
Villorita cyprinoides	2000		1
Cadmium			
TestSpecies	EC50		Total
Acartia simplex	1370		1
Acartia spinicauda	50		1
Acartia tonsa	122		1
Allorchestes compressa	300		1
Argopecten irradians	530		1
Artemia salina	1000		1
Asterias forbesi	820		1
Balanus improvisus	160		1
Callianassa australiensis	490		1
Callinectes sapidus	320		1
Capitella capitata	220		1
Carcinus maenas	4100		1
Charybdis feriatus	250		1
Crangon crangon	350		1
Crangon septemspinosa	320		1
Crassostrea gigas	22.5		1
Crassostrea rhizophorae	900		1
Crassostrea virginica	3800		1
Ctenodrilus serratus	2730		1
Cyprinodon variegatus	15900		1
Dinophilus gyrociliatus	2500		1
Ditylum brightwelli	60		1
Enoplus brevis	10		1
Enoplus communis	10		1
Eurypanopeus depressus	4900		1
Eurytemora affinis	60		1
Fundulus heteroclitus	7800		1
Fundulus majalis	21000		1
Homarus americanus	78		1
Idotea balthica	30		1
Ilyanassa obsoleta	112.4		1
Marinogammarus obtusatus	3.5		1
Menidia menidia	540		1
Morone saxatilis	75		1

Test species	EC50	StDev	number
Mugil cephalus	7079		1
Mya arenaria	150		1
Mysidopsis bahia	11.3		1
Mysidopsis bigelowi	14.8		1
Mytilus edulis	700		1
Nassarius obsoletus	10500		1
Neanthes vaali	6400		1
Neomysis americana	20		1
Nereis arenaceodentata	3000		1
Nereis virens	11000		1
Nitocra spinipes	40		1
Ophryotrocha diadema	2000		1
Ophryotrocha labronica	1000		1
Pagurus longicarpus	70		1
Palaemon sp	1850		1
Palaemonetes pugio	1000		1
Palaemonetes vulgaris	120		1
Paracalanus parvus	2710		1
Paragrapsus gaimardii	15700		1
Paragrapsus quadridentatus	490		1
Penaeus duorarum	4600		1
Penaeus indicus	2070		1
Portunus pelagicus	380		1
Portunus sanguinolentus	250		1
Pseudopleuronectes americanus	1000		1
Scorpaena guttata	62000		1
Scutellidium sp	660		1
Scylla serrata	18000		1
Tautogolabrus adspersus	25900		1
Thymallus arcticus	600		1
Tigriopus brevicornis	24.5		1
Tisbe holothuriae	333		1
Tortanus forcipatus	130		1
Uca pugilator	2900		1
Urosalpinx cinerea	6600		1

Appendix C FATE DATA

Substance	Molecular weight [g.mole^{-1}] (MOLW)	Reference
Benzene	78.11	Weast (1983)
Biphenyl	154.21	Weast (1983)
Cadmium	112.41	Weast (1983)
Chromium	51.996	Weast (1983)
Ethylbenzene	106.16	Weast (1983)
Phenanthrene	178.23	Weast (1983)
Phenol	94.113	Weast (1983)
Fluoranthene	202.26	Weast (1983)
Fluorene	166.22	Weast (1983)
Glycol	62.068	Weast (1983)
Mercury	200.59	Weast (1983)
Lead	207.2	Weast (1983)
Methanol	32.04	Weast (1983)
Naphthalene	128.18	Weast (1983)
Nickel	58.69	Weast (1983)
Oil	200	Evers *et al.* (1997)
Toluene	92.14	Weast (1983)
o-Xylene	106.17	Weast (1983)
m-Xylene	106.17	Weast (1983)
p-Xylene	106.17	Weast (1983)
Xylene	*106.17*	
Zinc	65.39	Weast (1983)

Substance	Vapour Pressure [Pa] (VP)	temp	Reference
Benzene	10108	20°	Richardson&Gangolli (1992)
Cadmium			
Chromium			
Ethylbenzene	944.3	20°	Jorgensen et al. (1991)
Fluoranthene	0.000133	20°	Richardson&Gangolli (1992)
Fluorene	1330	146°	Richardson&Gangolli (1992)
Glycol	6.65	20°	Richardson&Gangolli (1992)
glycol	0.079	20°	EC (1996)
glycol	0.082	20°	EC (1996)
glycol	0.1	20°	EC (1996)
glycol	0.067	20°	EC (1996)
Lead			
Mercury			
Methanol	13300	21.2°	Richardson&Gangolli (1992)
m-Xylene	851.2	20°	EC (1996)

Substance	Vapour Pressure [Pa] (VP)	temp	Reference
Naphthalene	6.65	20°	EC (1996)
Nickel			
Oil	26150		Koops (1992)
o-Xylene	691.6	20°	EC (1996)
Phenanthrene	0.0904	20°	Verschueren (1996)
Phenol	26.6	20°	Verschueren (1996)
p-Xylene	904.4	20°	EC (1996)
Toluene	2979.2	20°	EC (1996)
Xylene	815.7		EC (1996)
Zinc			

Substance	watersolubility [$g.l^{-1}$] (SOL)	Reference
Benzene	1.78E+00	ChemFinder
Cadmium		
Chromium		
Ethylbenzene	1.52E-01	Jorgensen et al. (1991)
Ethylbenzene	1.52E-01	Richardson & Gangolli (1992-'96)
Phenanthrene	1.6E-03	Richardson & Gangolli (1992-'96)
Phenol	0.828	ChemFinder
Fluoranthene	2.30E-04	Richardson & Gangolli (1992-'96)
Fluorene	1.8E-03	Richardson & Gangolli (1992-'96)
Glycol	>100	ChemFinder
Mercury	2.00E-05	Jorgensen et al. (1991)
Lead		
Methanol	>	ChemFinder
Naphthalene	0.031	ChemFinder
Naphthalene	1.50E-06	Jorgensen et al. (1991)
Naphthalene	1.25E-02	Jorgensen et al. (1991)
Naphthalene	2.10E-02	Jorgensen et al. (1991)
Naphthalene	2.20E-02	Jorgensen et al. (1991)
Naphthalene	3.17E-02	Jorgensen et al. (1991)
Naphthalene	3.30E-02	Jorgensen et al. (1991)
Nickel		
Oil	9.00E-07	Jorgensen et al. (1991)
Oil	1.00E-06	Jorgensen et al. (1991)
Oil	2.00E-05	Jorgensen et al. (1991)
Oil	1.10E-04	Jorgensen et al. (1991)
Oil	3.00E-03	Jorgensen et al. (1991)
Oil	5.00E-03	Jorgensen et al. (1991)
Toluene	0.526	ChemFinder
Xylene	0.175	ChemFinder

Substance	watersolubility [g.l^{-1}] (SOL)	Reference
o-Xylene	1.75E-01	Jorgensen et al. (1991)
m-Xylene	1.62E-01	ChemFinder
p-Xylene	1.85E-01	ChemFinder
Zinc		

Substance	Log Kow [-]	Reference
Benzene	2.13	SRC (1997)
Cadmium		
Chromium		
Ethylbenzene	3.15	SRC (1997)
Phenanthrene	4.46	SRC (1997)
Phenanthrene	4.57	Polder et al. (1994)
Phenol	1.46	SRC (1997)
Fluoranthene	5.16	SRC (1997)
Fluorene	4.18	SRC (1997)
Glycol	-1.36	SRC (1997)
Mercury		
Lead		
Methanol	-0.77	SRC (1997)
Naphthalene	3.3	SRC (1997)
Nickel		
Oil	6.3	Evers et al. (1997)
Toluene	2.73	SRC (1997)
o-Xylene	3.12	SRC (1997)
m-Xylene	3.2	SRC (1997)
p-Xylene	2.73	SRC (1997)
Zinc		

Substance	Meltingpoint [°C] (TEMPmelt)	Reference: ChemFinder
Benzene	5.5	
Cadmium		
Chromium		
Ethylbenzene	-95	
Phenanthrene	99.5	
Phenol	40.5	
Fluoranthene	110.8	
Fluorene	116	
Glycol	-13	
Mercury		
Lead		
Methanol	-98	
Naphthalene	80.6	
Nickel		

Substance	Meltingpoint [°C] (TEMPmelt)	Reference: ChemFinder
Oil		
Toluene	-93	
Xylene	-50	
o-Xylene	-25.2	
m-Xylene	-47.87	
p-Xylene	13.3	
Zinc		

Substance	Henry constant [$Pa.m^3.mole^{-1}$] (HENRY)	Reference
Benzene	506.63	Sander (1998)
Cadmium		
Chromium		
Ethylbenzene	779.42	Sander (1998)
Phenanthrene	3.4940	Sander (1998)
Phenol	0.04053	Sander (1998)
Fluoranthene	220.27	Sander (1998)
Fluorene	9.2114	Sander (1998)
Glycol	0.0059603	Sander (1998)
Mercury		
Lead		
Methanol	0.46057	Sander (1998)
Naphthalene	48.25	Sander (1998)
Nickel		
Oil**	100	
Toluene	633.28	Sander (1998)
Xylene	605.14	
o-Xylene	507	Sander (1998)
m-Xylene	675	Sander (1998)
p-Xylene	633	Sander (1998)
Zinc		

Substance	Photodegr. $DT_{50photo_{air}}$ [hours]high	Photodegr. $DT_{50photo_{air}}$ [hours]low	Reference Howard et al. (1991)
Benzene	501	50.1	
Cadmium			
Chromium			
Ethylbenzene	85.6	8.56	
Phenanthrene	20.1	2.01	
Phenol	22.8	2.28	
Fluoranthene	20.2	2.02	
Fluorene	68.1	6.81	
Glycol	83	8.3	

Substance	Photodegr. $DT_{50}photo_{air}$ [hours]high	Photodegr. $DT_{50}photo_{air}$ [hours]low	Reference Howard et al. (1991)
Mercury			
Lead			
Methanol	713	71	
Naphthalene	29.6	2.96	
Nickel			
Oil			
Toluene	104	10	
o-Xylene	44	4.4	
m-Xylene	26	2.6	
p-Xylene	42	4.2	
Zinc			

Substance	Biodegr. Water T½ [hours] high	Biodegr. Water T½ [hours] low	Reference Howard et al. (1991)
Benzene	384	120	
Cadmium			
Chromium			
Ethylbenzene	240	72	
Phenanthrene	4800	384	
Phenol	84	6	
Fluoranthene	10560	3360	
Fluorene	1440	768	
Glycol	288	48	
Mercury			
Lead			
Methanol	168	24	
Naphthalene	480	12	
Nickel			
Oil			
Toluene	528	96	
o-Xylene	672	168	
m-Xylene	672	168	
p-Xylene	672	168	
Zinc			

Substance	Biodegr. T½Soil [hours] high	Biodegr. T½Soil [hours] low	Reference Howard et al. (1991)
Benzene	384	120	
Cadmium			
Chromium			
Ethylbenzene	240	72	
Phenanthrene	4800	384	
Phenol	240	24	
Fluoranthene	10560	3360	
Fluorene	1440	786	
Glycol	288	48	
Mercury			
Lead			
Methanol	168	24	
Naphthalene	1152	398	
Nickel			
Oil	146		Evers et al. (1997)
Toluene	528	96	
o-Xylene	672	168	
m-Xylene	672	168	
p-Xylene	672	168	
Zinc			

Substance	BCF Plant leaves [mg.kg ds^{-1}].[mg.kg ds^{-1}]$^{-1}$	Reference: Berg (1995)
Benzene		
Cadmium	0.15	
Chromium	0.002	
Ethylbenzene		
Phenanthrene		
Phenanthrene		
Phenol		
Fluoranthene		
Fluorene		
Glycol		
Mercury	0.015	
Lead	0.001	
Methanol		
Naphthalene		
Naphthalene		
Nickel	0.07	
Oil**		
Toluene		
Xylene		
o-Xylene		
m-Xylene		
p-Xylene		
Zinc	0.1	

Substance	BCF cattle meat [$d.kg^{-1}$]	BCF cattle milk [$d.kg^{-1}$]	Reference: Ng (1982)
Benzene			
Cadmium	$7.2\ 10^{-4}$	$1.5\ 10^{-3}$	
Chromium	$9.2\ 10^{-3}$	$1.1\ 10^{-3}$	
Ethylbenzene			
Phenanthrene			
Phenanthrene			
Phenol			
Fluoranthene			
Fluorene			
Glycol			
Mercury	7.1 10-3 **	$4.7\ 10^{-4}$	**Jager et al, 1994
Lead	$1.0\ 10^{-4}$	$2.6\ 10^{-4}$	
Methanol			
Naphthalene			
Naphthalene			
Nickel	$2.0\ 10^{-3}$	$1.0\ 10^{-3}$	

Substance	BCF cattle meat [d.kg^{-1}]	BCF cattle milk [d.kg^{-1}]	Reference: Ng (1982)
Oil**			
Toluene			
Xylene			
o-Xylene			
m-Xylene			
p-Xylene			
Zinc	1.2 10^{-1}	1.0 10^{-2}	

Substance	Kd soil [l.kg^{-1}]	Reference: Tukkers & Roelofs (1985)
Benzene		
Cadmium	1940	
Chromium	33120	
Ethylbenzene		
Phenanthrene		
Phenanthrene		
Phenol		
Fluoranthene		
Fluorene		
Glycol		
Mercury	5600	
Lead	14020	
Methanol		
Naphthalene		
Naphthalene		
Nickel	1700	
Oil**		
Toluene		
Xylene		
o-Xylene		
m-Xylene		
p-Xylene		
Zinc	1890	

Substance	Kd susp. Matterl [l.kg^{-1}]	Reference: IAEA (1985)
Benzene		
Cadmium	5 10^{3}	
Chromium	5 10^{4}	
Ethylbenzene		
Phenanthrene		
Phenanthrene		
Phenol		
Fluoranthene		
Fluorene		

Substance	Kd susp. Matterl [l.kg^{-1}]	Reference: IAEA (1985)
Glycol		
Mercury	5 10^3	
Lead	3 10^7	
Methanol		
Naphthalene		
Naphthalene		
Nickel	1 10^6	
Oil**		
Toluene		
Xylene		
o-Xylene		
m-Xylene		
p-Xylene		
Zinc	2 10^5	

Appendix D FORMULARIUM

General indications

[regional]	referring to the regional system (The Netherlands)
[continental]	referring to the (global) continental system
[northsea]	referring to the North Sea system
[atlantic]	referring to the (global) oceanic system*

* For historical reasons, the oceanic system is referred to as the 'atlantic' system in the REIMSEA model.

DIFFUSIVE AND ADVECTIVE FLOWS BETWEEN MEDIA

Flows between sea air and seawater (deposition from air)

CONjunge	constant of Junge equation	0.173	Pa·m
SURFaersea	surface area of aerosol particles in air above seawater	$1.5 \cdot 10^{-4}$	
VP	vapour pressure	[1]	Pa
Fass_aersea	fraction of the chemical associated with aerosol particles in air above seawater	(1)	-
HENRY	Henry's law constant	[1]	$Pa \cdot m^3 \cdot mol^{-1}$
R	gas constant	8.314	$Pa \cdot m^3 \cdot mol^{-1} \cdot K^{-1}$
TEMPsea	temperature at the air-water interface	282	K
K_airseawater	air-seawater partition coefficient	(2)	$m_{water}^3 \cdot m_{air}^{-3}$
kaw_water	partial mass transfer coefficient at the water side of the air-water interface	$1.39 \cdot 10^{-5}$	$m_{water}^3 \cdot s^{-1}$
kaw_air	partial mass transfer coefficient at the air side of the air-water interface	$1.39 \cdot 10^{-3}$	$m_{air}^3 \cdot s^{-1}$
GASABS_seawater	overall mass transfer coefficient for gas absorption accross the air-seawater interface, referenced to air	(3)	$m_{air}^3 \cdot s^{-1}$

SYSTEMAREA[northsea]	total area of the North Sea system	$0.55 \cdot 10^{12}$	m^2
Farea_seawater[northsea]	fraction of North Sea area that is seawater	1	-
AREA_seawater[northsea]	area of North Sea seawater compartment	(4)	m^2
DIFF(northsea, air), (northsea, seawater)	transport coefficient for gasabsorption by the seawater compartment in the North Sea system	(5)	$m_{air}^3 \cdot s^{-1}$
SYSTEMAREA[atlantic]	total area of the oceanic system	$3.28 \cdot 10^{14}$	m^2
Farea_seawater[atlantic]	fraction of oceanic area that is seawater	1	-
AREA_seawater[atlantic]	area of oceanic seawater compartment	(6)	m^2
DIFF(atlantic, air), (atlantic, seawater)	transport coefficient for gasabsorption by the North Sea air compartment	(7)	$m_{air}^3 \cdot s^{-1}$
VOLAT_seawater	overall mass transfer coefficient for volatilization accross the air-seawater interface, referenced to water	(8)	$m_{water}^3 \cdot s^{-1}$
DIFF(northsea, seawater), (northsea, air)	transport coefficient for volatilization from the North Sea seawater compartment	(9)	$m_{water}^3 \cdot s^{-1}$
DIFF(atlantic, seawater), (atlantic, air)	transport coefficient for volatilization from the oceanic seawater compartment	(10)	$m_{water}^3 \cdot s^{-1}$
DEPRATE_aer	deposition velocity of the aerosol particles (with which the chemical is associated)	0.001	$m_{air} \cdot s^{-1}$
DRYDEP_aersea	mass transfer coefficient for dry deposition of aerosol-associated chemical in air above seawater	(11)	$m_{air}^3 \cdot s^{-1}$
RAINRATE[northsea]	rate of wet precipitation in the North Sea system	$1.9 \cdot 10^{-8}$	$m_{rain} \cdot s^{-1}$
SCAVratiosea	scavenging ratio (quotient of the total concentration in rain and the total concentration in air) of the chemical in air above seawater	(12)	$m_{air}^3 \cdot m_{water}^{-3}$
WASHOUT[northsea]	mass transfer coefficient for wet atmospheric deposition in the North Sea system	(13)	$m_{air}^3 \cdot s^{-1}$
ADV(northsea, air), (northsea, seawater)	transport coefficient for advective flows from air to the seawater in the North Sea system	(14)	$m_{water}^3 \cdot s^{-1}$
RAINRATE[atlantic]	rate of wet precipitation in the atlantic system	$1.9 \cdot 10^{-8}$	$m_{rain} \cdot s^{-1}$
WASHOUT[atlantic]	mass transfer coefficient for wet atmospheric deposition in	(15)	$m_{air}^3 \cdot s^{-1}$

	the oceanic system		
ADV(atlantic, air), (atlantic, seawater)	transport coefficient for advective flows from air to seawater in the oceanic system	(16)	$m_{water}^3 \cdot s^{-1}$

[1] Substance property

$$Fass_aersea = (CONjunge*SURFaersea)/(VP+CONjung*SURFaersea) \quad (1)$$

$$K_airseawater = HENRY/(R*TEMPsea) \quad (2)$$

$$GASABS_seawater = (1-Fass_aer)/((K_airseawater/kaw_water)+(1/kaw_air)) \quad (3)$$

$$AREA_seawater[northsea] = SYSTEMAREA[northsea]*Farea_seawater[northsea] \quad (4)$$

$$DIFF(northsea, air), (northsea, seawater) = GASABS_seawater*AREA_seawater[northsea]) \quad (5)$$

$$AREA_seawater[atlantic] = SYSTEMAREA[atlantic]*Farea_seawater[atlantic] \quad (6)$$

$$DIFF(atlantic, air), (atlantic, seawater) = GASABS_seawater*AREA_seawater[atlantic]) \quad (7)$$

$$VOLAT_seawater = GASABS_seawater/(1-Fass_aersea)*K_airseawater = 1/((1/kaw_water)+(1/(kaw_air*K_airseawater))) \quad (8)$$

$$DIFF(northsea, seawater), (northsea, air) = VOLAT_seawater*AREA_seawater[northsea]) \quad (9)$$

$$DIFF(atlantic, seawater), (atlantic, air) = VOLAT_seawater*AREA_seawater[atlantic]) \quad (10)$$

$$DRYDEP_aersea = DEPRATE_aer*Fass_aersea \quad (11)$$

$$SCAVratiosea = ((1-Fass_aersea)/K_airseawater)+Fass_aersea*2*10^5 \quad (12)$$

WASHOUT[northsea] = RAINRATE[northsea]*SCAVratiosea (13)

ADV(northsea, air), (northsea, seawater) = (DRYDEP_aersea+WASHOUT[northsea])*AREA_seawater[northsea] (14)

WASHOUT[atlantic] = RAINRATE[atlantic]*SCAVratiosea (15)

ADV(atlantic, air), (atlantic, seawater) = (DRYDEP_aersea+WASHOUT[atlantic])*AREA_seawater[atlantic] (16)

Flows between seawater and sea biota

AREA_seawater[northsea]	area of North Sea seawater compartment	(4)	m^2
DEPTH_seawater[northsea]	depth of North Sea seawater compartment	90	m
V_seawater[northsea]	volume of North Sea seawater compartment	(17)	m^3
BIOCONC_seawater	concentration of biota in seawater	0.001	$kg_{dry\ biota} \cdot m_{water}^{-3}$
Fwater_bio	volume fraction water in biota	0.95	$m_{water}^3 \cdot m_{wet\ biota}^{-3}$
RHOsolid	density of the solid phase	2500	$kg_{solid} \cdot m_{solid}^{-3}$
V_seabio[northsea]	volume of the North Sea biota compartment	(18)	m^3
Kow	octanol-water partition coefficient	1	-
EQUtime_bio	equilibrium half-time for water and biota	(19)	s
DIFF(northsea, seabio), (northsea, seawater)	transport coefficient for elimination from biota in the North Sea system	(20)	
AREA_seawater[atlantic]	area of oceanic seawater compartment	(6)	
DEPTH_seawater[atlantic]	depth of Oceanic seawater compartment	100	
V_seawater[atlantic]	volume of Oceanic seawater compartment	(21)	m^3
V_seabio[atlantic]	volume of the Oceanic biota compartment	(22)	m^3
DIFF(atlantic, seabio), (atlantic, seawater)	transport coefficient for elimination from biota in the oceanic system	(23)	$m_{bio}^3 \cdot s^{-1}$
Ffat_fish	volume fraction of fat in fish	0.05	$m_{fat}^3 \cdot m_{wet\ fish}^{-3}$
RHO_bio	bulk density of aquatic biota	1000	$kg_{wet\ biota} \cdot m_{wet}$

			$biota^{-3}$
BCF_fish	bioconcentration factor for fish	(24)	$(kg_{chem} \cdot kg_{wet\ biota}^{-1} / (kg_{chem} \cdot m_{water}^{-3})$
K_fishwater	fish-water partition coefficient	(25)	$m_{water}^{3} \cdot m_{biota}^{-3}$
DIFF(northsea, seawater), (northsea, seabio)	transport coefficient for uptake by biota in the North Sea system	(26)	$m_{bio}^{3} \cdot s^{-1}$
DIFF(atlantic, seawater), (atlantic, seabio)	transport coefficient for uptake by biota in the oceanic system	(27)	$m_{water}^{3} \cdot s^{-1}$

[1] Substance property

V_seawater[northsea] = AREA_seawater[northsea]*DEPTH_seawater[northsea] (17)

V_seabio[northsea] = V_seawater[northsea]*BIOCONC_seawater/((1-Fwater_bio)*RHOsolid) (18)

*EQUtime_bio = (100+Kow/1000)*3600* (19)

DIFF(northsea, seabio), (northsea, seawater) = (ln(2.0)/EQUtime_bio)*V_seabio[northsea]) (20)

V_seawater[atlantic] = AREA_seawater[atlantic]*DEPTH_seawater[atlantic] (21)

V_seabio[atlantic] = V_seawater[atlantic]*BIOCONC_seawater/((1-Fwater_bio)*RHOsolid) (22)

DIFF(atlantic, seabio), (atlantic, seawater) = (ln(2.0)/EQUtime_bio)*V_seabio[atlantic]) (23)

*BCF_fish = (Ffat_fish*Kow)/RHO_bio* (24)

*K_fishwater = BCF_fish*RHO_bio* (25)

DIFF(northsea, seawater), (northsea, seabio) = DIFF(northsea, seabio), (northsea, seawater))*K_fishwater (26)

DIFF(atlantic, seawater), (atlantic, seabio) = DIFF(atlantic, seabio), (atlantic, seawater))*K_fishwater (27)

Flows between seawater and sea sediment

kws_water	partial mass transfer coefficient at the water-side of the sediment-water interface	$2.78 \cdot 10^{-6}$	$m_{water}^3 \cdot s^{-1}$
kws_sed	partial mass transfer coefficient at the porewater-side of the sediment-water interface	$2.78 \cdot 10^{-8}$	$m_{porewater}^3 \cdot s^{-1}$
ADSORB_seased	overall mass transfer coefficient for adsorption accross the sediment-water interface, referenced to water	(28)	$m_{water}^3 \cdot s^{-1}$
a	Karickhoff parameter	0.411	$dm_{water}^3 \cdot kg_{oc}^{-1}$
Foc_sed	fraction organic carbon in sediment	0.05	$kg_{oc} \cdot kg_{solid}^{-1}$
Kow	octanol-water partition coefficient	1	-
Kp_sed	solids-water partition coefficient in sediment	(29)	$m_{water}^3 \cdot kg_{solid}^{-1}$
Fwater_sed	volume fraction of water in sediment	0.8	$m_{water}^3 \cdot m_{sed}^{-3}$
Fsolid_sed	volume fraction of solids in sediment	0.2	$m_{solid}^3 \cdot m_{sed}^{-3}$
RHOsolid	density of the solid phase	2500	$kg_{solid} \cdot m_{solid}^3$
K_sedwater	sediment-water partition coefficient	(30)	$m_{water}^3 \cdot m_{sed}^{-3}$
DESORB_sed	overall mass transfer coefficient for desorption accross the sediment-water interface, referenced to water	(31)	$m_{sed}^3 \cdot s^{-1}$
AREA_seawater[northsea]	area of North Sea seawater compartment	(4)	m^2
DIFF(northsea, seased), (northsea, seawater)	transport coefficient for desorption from the North Sea sea sediment compartment	(32)	$m_{sea\ sed}^3 \cdot s^{-1}$
DIFF(northsea, seawater), (northsea, seased)	transport coefficient for adsorption to the North Sea sea sediment compartment	(33)	$m_{seawater}^3 \cdot s^{-1}$
V_seawater[atlantic]	volume of the oceanic seawater compartment	(21)	m^3
TAU_surfocean[atlantic]	residence time of chemical in oceanic mixed surface layer	1	s
ADV(atlantic, seawater), (atlantic, seased)	transport coefficient for advective water flows from	(34)	$m_{water}^3 \cdot s^{-1}$

	oceanic seawater to oceanic sediment		

[1] Substance property

$$ADSORB_sed = 1.0/(1.0/kws_water+1.0/kws_sed) \quad (28)$$

$$Kp_sed = (a*Foc_sed*Kow)/1000 \quad (29)$$

$$K_sedwater = Fwater_sed+Fsolid_sed*Kp_sed*RHOsolid \quad (30)$$

$$DESORB_sed = ADSORB_sed/K_sedwater \quad (31)$$

DIFF(northsea, seased), (northsea, seawater) = DESORB_sed*AREA_seawater[northsea]) (32)

DIFF(northsea, seawater), (northsea, seased) = ADSORB_seased*AREA_seawater[northsea]) (33)

metals

ADV(atlantic, seawater), (atlantic, seased) = V_seawater[atlantic]/TAU_surfocean[atlantic] (34)

Flows between seawater and sea suspended matter

V_seawater[northsea]	volume of the North sea seawater compartment	(17)	m^3
SUSPCONC_seawater[northsea]	concentration of suspended matter in Northsea seawater	0.03	$kg_{solids} \cdot m_{seawater}^{-3}$
Fwater_susp	volume fraction of water in suspended matter	0.9	$m_{water}^3 \cdot m_{susp}^{-3}$
RHOsolid	density of the solid phase	2500	$kg_{solid} \cdot m_{solid}^{-3}$
V_seasusp[northsea]	volume of the sea suspended matter compartment of the North Sea system	(35)	m^3
EQUtime_susp	equilibration time for seawater and sea suspended particles	$3.6 \cdot 10^4$	s
DIFF(northsea, seasusp), (northsea, seawater)	transport coefficient for desorption from the North Sea sea suspended matter compartment	(36)	$m_{sea\ susp}^3 \cdot s^{-1}$

V_seawater[atlantic]	volume of the oceanic seawater compartment	(21)	m^3
SUSPCONC_seawater[atlantic]	concentration of suspended matter in oceanic seawater	0.00009	$kg_{sobds} \cdot m_{seawater}^{-3}$
V_seasusp[atlantic]	volume of the sea suspended matter compartment of the oceanic system	(37)	m^3
DIFF(atlantic, seasusp), (atlantic, seawater)	transport coefficient for desorption from the oceanic sea suspended matter compartment	(38)	$m_{sea\ susp.}^{3} \cdot s^{-1}$
Fsolid_susp	volume fraction of solid in suspended matter	0.1	$m_{solid}^{3} \cdot m_{susp}^{-3}$
a	Karickhoff parameter	0.411	$dm_{water}^{3} \cdot kg_{oc}^{-1}$
Foc_sed	fraction organic carbon in sediment	0.05	$kg_{oc} \cdot kg_{solid}^{-1}$
Kow	octanol-water partition coefficient	[1]	-
Kp_susp	solids-water partition coefficient in ssuspended matter	(39)	$m_{water}^{3} \cdot kg_{susp}^{-1}$
K_suspwater	suspended matter-seawater partition coefficient	(40)	$m_{water}^{3} \cdot m_{susp}^{-3}$
DIFF(northsea, seawater), (northsea, seasusp)	transport coefficient for adsorption to the North Sea sea suspended matter compartment	(41)	$m_{seawater.}^{3} \cdot s^{-1}$
DIFF(atlantic, seawater), (atlantic, seasusp)	transport coefficient for adsorption to the oceanic sea suspended matter compartment	(42)	$m_{seawater.}^{3} \cdot s^{-1}$

[1] Substance property

V_seasusp[northsea] = V_seawater[northsea]*SUSPCONC_seawater[northsea]/((1.0-Fwater_susp)*RHOsolid) (35)

DIFF(northsea, seasusp), (northsea, seawater) = ln(2.0)/EQUtime_susp*V_seasusp[northsea] (36)

V_seasusp[atlantic] = V_seawater[atlantic]*SUSPCONC_seawater[atlantic]/((1.0-Fwater_susp)*RHOsolid) (37)

DIFF(atlantic, seasusp), (atlantic, seawater) = ln(2.0)/EQUtime_susp*V_seasusp[atlantic] (38)

$Kp_susp=(a*Foc_susp*Kow)/1000$ (39)

$K_suspwater = Fwater_susp+Fsolid_susp \cdot Kp_susp \cdot RHOsolid$ (40)

DIFF(northsea, seawater), (northsea, seasusp) = DIFF(northsea, seasusp), (northsea, seawater)*K_suspwater (41)

DIFF(atlantic, seawater), (atlantic, seasusp) = DIFF(atlantic, seasusp), (atlantic, seawater)*K_suspwater (42)

Flows between sea suspended matter and sea sediment (sedimentation)

DEPOSITION_seasusp[northsea]	deposition velocity of North Sea sea suspended particles	1400	$kg_{seasusp} \cdot s^{-1}$
Fsolid_sed	volume fraction solids of sediment	0.2	-
RHOsolid	density of the solid phase of sediment	2500	$kg_{solid} \cdot m_{solid}^{-3}$
AREA_seawater[northsea]	area of the North Sea seawater compartment	(4)	m^2
NETseasedrate[northsea]	net sedimentation rate in North Sea seawater	(43)	$m_{seased} \cdot s^{-1}$
EROSION_seased[northsea]	rate of erosion of North Sea seafloor and coast	420	$kg_{solid} \cdot s^{-1}$
RESUSPsearate[northsea]	resuspension rate in North Sea seawater	(44)	$m_{seased} \cdot s^{-1}$
GROSSseasedrate[northsea]	gross sedimentation rate in North Sea seawater	(45)	$m_{seased} \cdot s^{-1}$
Fsolid_susp	volume fraction solids of suspended matter	0.1	-
ADV(northsea, seasusp), (northsea, seased)	transport coefficient for advective suspended matter flows from sea suspended matter to sea sediment in the North Sea system	(46)	$m_{seasusp}^3 \cdot s^{-1}$
ADV(northsea, seased), (northsea, seasusp)	transport coefficient for advective suspended matter flows from sea sediment to sea suspended matter in the North Sea system	(47)	$m_{seased} \cdot s^{-1}$
SUSPCONC_seawater[atlantic]	concentration of suspended matter in the oceanic seawater	0.00009	$kg_{solid} \cdot m_{seawater}^{-3}$
SUSPCONC_seawater[northsea]	concentration of suspended matter in North Sea seawater	0.03	$kg_{solid} \cdot m_{seawater}^{-3}$
SETTLvelocity_seasusp[atlantic]	settling velocity of suspended particles in oceanic seawater	$1.85 \cdot 10^{-6}$	$m_{seawater} \cdot s^{-1}$
GROSSseasedrate[atlantic]	gross sedimentation rate in oceanic seawater	(48)	$m_{seased} \cdot s^{-1}$
V_seasusp[atlantic]	volume of the oceanic sea suspended matter compartment	(37)	$m_{seasusp}^3$
TAUsurf_ocean[atlantic]	residence time of chemical in oceanic mixed surface layer	1	S
ADV(atlantic, seasusp), (atlantic, seased)	transport coefficient for advective suspended matter flows from sea suspended matter to sea sediment in the oceanic system	(49), (51)	$m_{seasusp} \cdot s^{-1}$

[1] Substance property

NORTH SEA

NETseasedrate[northsea] = DEPOSITION_seasusp[northsea]/(Fsolid_sed*RHOsolid*AREA_seawater[northsea]) (43)

RESUSPsearate[northsea] = EROSION_seased[northsea]/(Fsolid_sed*RHOsolid*AREA_seawater[northsea]) (44)

GROSSseasedrate[northsea] = NETseasedrate[northsea]+RESUSPsearate[northsea] (45)

ADV(northsea, seasusp), (northsea, seased) =
GROSSseasedrate[northsea]*(Fsolid_sed[northsea]/Fsolid_susp[northsea])*AREA_seawater[northsea]) (46)

ADV(northsea, seased), (northsea, seasusp) = RESUSPsearate[northsea]*AREA_seawater[northsea]) (47)

OCEANS

organics
GROSSseasedrate[atlantic] = (SETTLvelocity_seasusp[atlantic]*SUSPCONC_seawater[atlantic])/(Fsolid_sed*RHOsolid) (48)

ADV(atlantic, seasusp), (atlantic, seased) = GROSSseasedrate[atlantic]*(Fsolid_sed/Fsolid_susp)*AREA_seawater[atlantic]) (49)

metals
ADV(atlantic, seasusp), (atlantic, seased) = V_seasusp[atlantic]/TAU_surfocean[atlantic]) (50)

Flows between sea sediment and outside (burial)

NETseasedrate[northsea]	net sedimentation rate in the North Sea	(43)	$m_{seased} \cdot s^{-1}$
AREA_seawater[northsea]	area of a seawater compartment	(4)	m^2
ADV(northsea, seased), outside	transport coefficient for sediment burial in the North Sea system	(51)	$m_{seased} \cdot s^{-1}$

ADV(northsea, seased), outside = NETseasedrate[northsea]*AREA_seawater[northsea]) (51)

ADVECTIVE FLOWS BETWEEN REGIONS

Air flows between regions

SYSTEMAREA[regional]	total area of the Dutch system (air/water + air/soil interfaces)	$3.8 \cdot 10^{10}$	m^2
HEIGHT_air	atmospheric mixing height	1000	m
V_air[regional]	volume of the Dutch air compartment	(52)	m_{air}^3
WINDSPEED	average wind speed 10 m above the surface	5.8	$m \cdot s^{-1}$
TAU_air[regional]	residence time of air in the Dutch system	(53)	s
ADV(regional, air), (continental, air)	transport coefficient for advective air flows from the Dutch to the continental system	(54)	$m_{air}^3 \cdot s^{-1}$
ADV(continental air), (regional, air)	transport coefficient for advective air flows from the continental to the Dutch system	(55)	$m_{air}^3 \cdot s^{-1}$
ADV(regional air, northsea air)	transport coefficient for advective air flows from the Dutch to the North Sea system	(56)	$m_{air}^3 \cdot s^{-1}$
ADV(northsea, air), (regional, air)	transport coefficient for advective air flows from the North Sea to the Dutch system	(57)	$m_{air}^3 \cdot s^{-1}$
SYSTEMAREA[northsea]	total area of the North Sea system (air/water interface)	$0.55 \cdot 10^{12}$	m^2
V_air[northsea]	volume of the North Sea air compartment	(58)	m^3

ADV(northsea, air, atlantic, air)	transport coefficient for advective air flows from the Dutch to the oceanic system	(59)	$m_{air}^3 \cdot s^{-1}$
ADV(atlantic, air), (northsea, air)	transport coefficient for advective air flows from the oceanic to the Dutch system	(60)	$m_{air}^3 \cdot s^{-1}$
ADV(northsea, air), (continental, air)	transport coefficient for advective air flows from the North Sea to the continental system	(61)	$m_{air}^3 \cdot s^{-1}$
ADV(continental, air), (northsea, air)	transport coefficient for advective air flows from the coontinental to the North Sea system	(62)	$m_{air}^3 \cdot s^{-1}$
SYSTEMAREA[continental]	transport coefficient for advective air flows from the oceanic to the North Sea system	$3.28 \cdot 10^{14}$	m^2
V_air[continental]	volume of the oceanic air compartment	(63)	m^3
TAU_air[continental]	residence time of air in the oceanic system	(64)	s
ADV(continental, air), (atlantic, air)	transport coefficient for advective air flows from the continental to the oceanic system	(65)	$m_{air}^3 \cdot s^{-1}$
ADV(atlantic, air), (continental, air)	transport coefficient for advective air flows from the oceanic to the continental system	(66)	$m_{air}^3 \cdot s^{-1}$

*V_air[regional] = SYSTEMAREA[regional]*HEIGHT_air* (52)

*TAU_air[regional] = ((SYSTEMAREA[regional]*PI/4)E0.5)/WINDSPEED* (53)

ADV(regional, air), (continental, air) = 0.5*V_air[regional]/TAU_air[regional] (54)

ADV(continental air), (regional, air) = ADV(regional, air), (continental, air) (55)

ADV(regional air, northsea air) = 0.5*V_air[regional]/TAU_air[regional] (56)

ADV(northsea, air), (regional, air) = ADV(regional, air), (northsea, air) (57)

V_air[northsea] = SYSTEMAREA[northsea]*HEIGHT_air (58)

ADV(northsea, air, atlantic, air) = 0.2* V_air[northsea]/TAU_air[northsea]) (59)

ADV(atlantic, air), (northsea, air) = ADV(northsea, air), (atlantic, air) (60)

ADV(northsea, air), (continental, air) = V_air[northsea]/TAU_air[northsea])-ADV(northsea, air), (regional, air)-ADV(northsea, air), (atlantic, air) (61)

ADV(continental, air), (northsea, air) = ADV(northsea, air), (continental, air) (62)

*V_air[continental] = SYSTEMAREA[continental]*HEIGHT_air* *(63)*

*TAU_air[continental] = ((SYSTEMAREA[continental]*PI/4)E0.5)/WINDSPEED* *(64)*

ADV(continental, air), (atlantic, air) = V_air[continental]/TAU_air[continental]) -ADV(continental, air), (regional, air)-ADV(continental, air), (northsea, air) (65)

ADV(atlantic, air), (continental, air) = ADV(continental, air), (atlantic, air) (66)

Water flows between regions

SYSTEMAREA[regional]	total area of the Dutch system (air/water + air/soil interfaces)	$3.8 \cdot 10^{10}$	m^2
Farea_nat[regional]	fraction of regional area that is natural soil	0.415	
AREA_nat[regional]	area of Dutch natural soil compartment	(67)	m^2
Farea_agr[regional]	fraction of regional area that is agricultural soil	0.45	
AREA_agr[regional]	area of Dutch agricultural soil compartment	(68)	m^2
Farea_ind[regional]	fraction of regional area that is industrial soil	0.01	
AREA_ind[regional]	area of Dutch industrial soil compartment	(69)	m^2
Frunoff_soil[regional]	fraction of rain water that runs off soil	0.25	-
RAINRATE[regional]	average annual precipitation in the Dutch system	$2.22 \cdot 10^{-8}$	$m*s^{-1}$

WATERrunoff[regional]	total water run off from soil into the Dutch water compartment	(70)	$m_{water}^3 * s^{-1}$
INFLOW_water[regional, northsea]	sum of the discharges of streams flowing from the Dutch to the North Sea system	3113	$m_{water}^3 * s^{-1}$
CAPACITY_stp[regional]	total capacity of all STPs in the Dutch system	$1.0 \cdot 10^7$	eq
WASTEWinhab[regional]	wastewater per inhabitant	0.15	$m^3 * s^{-1} * eq^{-1}$
EFFLUENT_stp[regional]	total effluent discharges to the Dutch freshwater compartment	(71)	$m^3 * s^{-1}$
ADV(continental, water), (regional, water)	transport coefficient for advective water flows from the continental to the Dutch system	(72)	$m_{water}^3 \cdot s^{-1}$
ADV(regional, water), (northsea, seawater)	transport coefficient for advective water flows from the Dutch to the North Sea system	(73)	$m_{water}^3 \cdot s^{-1}$
INFLOW_seawater[northsea, atlantic]	sum of the seawater streams flowing from the North Sea to the oceanic system	$1.84 \cdot 10^6$	$m_{seawater}^3 * s^{-1}$
ADV(northsea, seawater), (atlantic, seawater)	transport coefficient for advective seawater flows from the North Sea to the oceanic system	(74)	$m_{water}^3 \cdot s^{-1}$
INFLOW_seawater[atlantic, northsea]	sum of the seawater streams flowing from the oceanic to the North Sea system	$1.84 \cdot 10^6$	$m_{seawater}^3 * s^{-1}$
ADV(atlantic, seawater), (northsea, seawater)	transport coefficient for advective seawater flows from the oceanic to the North Sea system	(75)	$m_{water}^3 \cdot s^{-1}$
INFLOW_water[continental, northsea]	sum of the discharges of streams flowing from the continental to the North Sea system	1876	$m_{water}^3 * s^{-1}$
ADV(continental, water), (northsea, seawater)	transport coefficient for advective water flows from the continental to the North Sea system	(76)	$m_{water}^3 \cdot s^{-1}$
INFLOW_water[continental, atlantic]	sum of the discharges of streams flowing from the continental to the oceanic system	$1.3 \cdot 10^6$	$m_{water}^3 * s^{-1}$
ADV(continental, water), (atlantic, seawater)	transport coefficient for advective water flows from the continental to the oceanic system	(77)	$m_{water}^3 \cdot s^{-1}$

*AREA_nat[regional] = SYSTEMAREA[regional]*Farea_nat[regional]* (67)

$AREA_agr[regional] = SYSTEMAREA[regional]*Farea_agr[regional]$ (68)

$AREA_ind[regional] = SYSTEMAREA[regional]*Farea_ind[regional]$ (69)

$WATERrunoff[regional] = Frunoff_soil*(AREA_nat[regional]+AREA_agr[regional]+AREA_ind[regional])*RAINRATE[regional]$ (70)

$EFFLUENT_stp[regional] = CAPACITY_stp[regional]*WASTEWinhab[regional]$ (71)

ADV(continental, water), (regional, water) = INFLOW_water[regional, northsea]-(EFFLUENT_stp[regional]+WATERrunoff[regional]) (72)

ADV(regional, water), (northsea, seawater) = INFLOW_water[regional, northsea] (73)

ADV(northsea, seawater), (atlantic, seawater) = INFLOW_seawater[northsea, atlantic] (74)

ADV(atlantic, seawater), (northsea, seawater) = INFLOW_seawater[atlantic, northsea] (75)

ADV(continental, water), (northsea, seawater) = INFLOW_water[continental, northsea] (76)

ADV(continental, water), (atlantic, seawater) = INFLOW_water[continental, atlantic] (77)

Suspended matter flows between regions

SYSTEMAREA[continental]	total area of the continental system	$1.5 \cdot 10^{14}$	m^2
Farea_water[continental]	fraction of continental area that is water	0.03	-
AREA_water[continental]	area of continental freshwater compartment	(78)	m^2
DEPTH_water[continental]	depth of continental freshwater compartment	3	m
V_water[continental]	volume of the continental water compartment	(79)	m^3
SUSPCONC_water[continental]	concentration of suspended matter in continental freshwater	0.056	$kg \cdot m^{-3}$

Fwater_susp	volume fraction of water in suspended matter	0.9	$m_{water}^3 \cdot m_{susp}^{-3}$
RHOsolid	density of the solid phase	2500	$kg_{solid} \cdot m_{solid}^3$
V_susp[continental]	volume of the continental suspended matter compartment	(80)	m^3
ADV(continental, water), (regional, water)	transport coefficient for advective water flows from the continental to the Dutch system	(72)	$m_{water}^3 \cdot s^{-1}$
ADV(continental, susp), (regional, susp)	transport coefficient for advective suspended matter flows from the continental to the Dutch system	(81)	$m_{susp.\ m.}^3 \cdot s^{-1}$
SYSTEMAREA[regional]	total area of the Dutch system (air/water + air/soil interfaces)	$3.8 \cdot 10^{10}$	m^2
Farea_water[regional]	fraction of Dutch area that is fresh water	0.125	-
AREA_water[regional]	area of regional freshwater compartment	(82)	m^2
V_water[regional]	volume of the Dutch water compartment	(83)	m^3
V_susp[regional]	volume of the Dutch suspended matter compartment	(84)	m^3
Fsusp_seased	fraction of freshwater suspended matter that is immediatly deposited on the seafloor when freshwater streams enter a marine system	0.9	-
ADV(regional, water), (northsea, seawater)	transport coefficient for advective water flows from the Dutch to the North Sea system	(73)	$m_{water}^3 \cdot s^{-1}$
ADV(regional, susp), (northsea, seasusp)	transport coefficient for advective suspended matter flows from the Dutch to the North Sea system	(85)	$m_{water}^3 \cdot s^{-1}$
ADV(continental, water), (northsea, seawater)	transport coefficient for advective water flows from the continental to the North Sea system	(76)	$m_{water}^3 \cdot s^{-1}$
ADV(continental, susp), (northsea, seasusp)	transport coefficient for advective suspended matter flows from the continental to the North Sea system	(86)	$m_{susp.\ m.}^{3*} s^{-1}$
ADV(continental, susp), (atlantic, seasusp)	transport coefficient for advective suspended matter flows from the continental to the oceanic system	(87)	
ADV(continental, water), (atlantic, seawater)	transport coefficient for advective water flows from the continental to the oceanic system	(77)	$m_{water}^3 \cdot s^{-1}$
INFLOW_seasusp[northsea, atlantic]	sum of the sea suspended matter streams flowing from the North Sea to the oceanic system	4.7	$m_{susp.\ m.}^{3*} s^{-1}$

ADV(northsea, seasusp), (atlantic, seasusp)	transport coefficient for advective suspended matter flows from the North Sea to the oceanic system	(88)	$m_{susp.\ m.}{}^{3}*s^{-1}$
INFLOW_seasusp[atlantic, northsea]	sum of the sea suspended matter streams flowing from the oceanic to the North Sea system	1.4	$m_{susp.\ m.}{}^{3}*s^{-1}$
ADV(atlantic, seasusp), (northsea, seasusp)	transport coefficient for advective suspended matter flows from the oceanic to the North Sea system	(89)	$m_{susp.\ m.}{}^{3}*s^{-1}$

*AREA_water[continental] = SYSTEMAREA[continental]*Farea_water[continental]* (78)

*V_water[continental] = AREA_water[continental]*DEPTH_water[continental]* (79)

V_susp[continental] = V_water[continental] SUSPCONC_water[continental]((1-Fwater_susp)*RHOsolid)* (80)

ADV(continental, susp), (regional, susp) = ADV(continental, water), (regional, water)*(V_susp[continental]/V_water[continental]) (81)

*AREA_water[regional] = SYSTEMAREA[regional]*Farea_water[regional]* (82)

*V_water[regional] = AREA_water[regional]*DEPTH_water[regional]* (83)

V_susp[regional] = V_water[regional] SUSPCONC_water[regional]((1-Fwater_susp)*RHOsolid)* (84)

ADV(regional, susp), (northsea, seasusp) = (1.0-Fsusp_seased)*ADV(regional, water), (northsea, seawater)*(V_susp[regional]/V_water[regional])) (85)

ADV(continental, susp), (northsea, seasusp) = (1.0-Fsusp_seased)*ADV(continental, water), (northsea, seawater)*(V_susp[continental]/V_water[continental])) (86)

ADV(continental, susp), (atlantic, seasusp) = (1.0-Fsusp_seased)*ADV(continental, water), (atlantic, seawater)*(V_susp[continental]/V_water[continental]) (87)

ADV(northsea, seasusp), (atlantic, seasusp) = INFLOW_seasusp[northsea, atlantic] (88)

ADV(atlantic, seasusp), (northsea, seasusp) = INFLOW_seasusp[atlantic, northsea] (89)

Suspended matter flows between regions, leading to immediate sedimentation

Fsusp_seased	fraction of freshwater suspended matter that is immediatly deposited on the seafloor when freshwater streams enter a marine system	0.9	-
ADV(regional, water), (northsea, seawater)	transport coefficient for advective water flows from the Dutch to the North Sea system	(73)	$m_{water}^3 \cdot s^{-1}$
V_susp[regional]	volume of the Dutch suspended matter compartment	(84)	m^3
V_water[regional]	volume of the water compartment of the Dutch system	(73)	m^3
ADV(regional, susp), (northsea, seased)	transport coefficient for advective suspended matter flows from the Dutch suspended matter to the North sea sediment compartment	(90)	$m_{water}^3 \cdot s^{-1}$
ADV(continental, water), (northsea, seawater)	transport coefficient for advective suspended matter flows from the continental suspended matter to the North sea sediment compartment	(76)	$m_{water}^3 \cdot s^{-1}$
V_susp[continental]	volume of the continental suspended matter compartment	(80)	m^3
V_water[continental]	volume of the continental water compartment	(79)	m^3
ADV(continental, susp), (northsea, seased)	transport coefficient for advective suspended matter flows from the Dutch suspended matter to the North sea sediment compartment	(91)	$m_{water}^3 \cdot s^{-1}$
ADV(continental, water), (atlantic, seawater)	transport coefficient for advective suspended matter flows from the continental suspended matter to the oceanic sediment compartment	(77)	$m_{water}^3 \cdot s^{-1}$
ADV(continental, susp), (atlantic, seased)	transport coefficient for advective suspended matter flows from the continental suspended matter to the oceanic sediment compartment	(92)	$m_{water}^3 \cdot s^{-1}$

ADV(regional, susp), (northsea, seased) = Fsusp_seased*ADV(regional, water), (northsea, seawater)*(V_susp[regional]/V_water[regional]) (90)

ADV(continental, susp), (northsea, seased) = Fsusp_seased*ADV(continental, water), (northsea, seawater)*(V_susp[continental]/V_water[continental]) (91)

ADV(continental, susp), (atlantic, seased) = Fsusp_seased*ADV(continental, water), (atlantic, seawater)*(V_susp[continental]/V_water[continental])) (92)

BIOAVAILABILITY

BIO_ecoseawater	bioavailability for ecosystems in seawater	(93),(94)	-
FREEIONseawater	relative amount of free ions in seawater	[1]	-
FREEIONtest	relative amount of free ions in test medium	[1]	-
BCF_fish	bioconcentration factor for fish	(24)	$(kg_{chem} \cdot kg_{wet\ biota}^{-1} / (kg_{chem} \cdot m_{water}^{-3})$
C(northsea, seawater)	concentration in North Sea seawater	[2]	$kg_{chem} \cdot m_{seawater}^{-3}$
C_seafish[northsea]	concentration in North Sea marine fish	(95)	
C(atlantic, seawater)	concentration in oceanic seawater	[2]	$kg_{chem} \cdot m_{seawater}^{-3}$
C_seafish[atlantic]	concentration in oceanic marine fish	(96)	
effectparameter(marinetox)	effect parameter for marine ecotoxicity	[1]	$kg_{chem} \cdot m_{seawater}^{-3}$
RCR[northsea]	risk characterization ratio for ecotoxicity in the North Sea system	(97)	-
RCR[atlantic]	risk characterization ratio for ecotoxicity in the North Sea system	(98)	-

[1] Substance property
[2] Model outcome

organics:

BIO_ecoseawater = 1 (93)

metals:

BIO_ecoseawater = FREEIONseawater/FREEIONtest (94)

general:

C_seafish[northsea] = BCF_fish*C(northsea, seawater)*BIO_ecoseawater (95)

C_seafish[atlantic] = BCF_fish*C(atlantic, seawater)*BIO_ecoseawater (96)

RCR[northsea] = BIO_ecoseawater*C(northsea, seawater)/effectparameter(marinetox) (97)

RCR[atlantic] = BIO_ecoseawater*C(atlantic, seawater)/effectparameter(marinetox) (98)

HUMAN CONSUMPTION

C_x[regional]	concentration in foodstuff *x* in the Dutch system	[2]	$kg_{chem} \cdot m_x^{-3}$
IH_drw	daily intake of drinking water	0.002	$m_{drinking\ water}^3 \cdot d^{-1}$
DOSE_drw[regional]	Dutch human dose through intake of drinking water	(99)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
BW	average human bodyweight	70	kg
C_fish[regional]	concentration of chemical in Dutch freshwater fish	[2]	$kg_{chem} \cdot m_{fish}^{-3}$
IH_freshfish[regional]	Dutch daily intake of freshwater fish	0.0005	$kg_{wet\ freshw.\ fish} \cdot d^{-1}$
DOSE_freshfish[regional]	Dutch human dose through intake of freshwater fish from the Dutch freshwater compartment	(100)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$

C_seafish[northsea]	concentration in North Sea marine fish	2	$kg_{chem} \cdot m_{seabio}^{-3}$
IH_northseafish[regional]	Dutch daily intake of North Sea marine fish	0.0072	$kg_{wet\ marine\ fish} \cdot d^{-1}$
DOSE_northseafish[regional]	Dutch human dose through intake of North Sea marine fish	(101)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
C_seafish[atlantic]	concentration in oceanic marine fish	2	$kg_{chem} \cdot m_{seabio}^{-3}$
IH_atlanticfish[regional]	Dutch daily intake of oceanic marine fish	0.0018	$kg_{wet\ marine\ fish} \cdot d^{-1}$
DOSE_atlanticfish[regional]	Dutch human dose through intake of oceanic marine fish	(102)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
IH_leafcrops	daily intake of leaf crops	0.349	$kg_{leaf\ crops} \cdot d^{-1}$
DOSE_leafcrops[[regional]	Dutch human dose through intake of leaf crops	(103)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
IH_rootcrops	daily intake of root crops	0.124	$kg_{root\ crops} \cdot d^{-1}$
DOSE_rootcrops[regional]	Dutch human dose through intake of root crops	(104)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
IH_meat	daily intake of meat	0.120	$kg_{meat} \cdot d^{-1}$
DOSE_meat[regional]	Dutch human dose through intake of meat	(105)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
IH_dairy	daily intake of dairy	0.378	$kg_{dairy} \cdot d^{-1}$
DOSE_dairy[regional]	Dutch human dose through intake of dairy	(106)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
DOSE_totoral[regional]	Dutch total human oral dose	(107)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
DOSE_drw[continental]	continental human dose through intake of drinking water	(108)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
IH_freshfish[continental]	continental daily intake of freshwater fish	0.001	$kg_{wet\ freshw.\ fish} \cdot d^{-1}$
DOSE_freshfish[continental]	continental human dose through intake of freshwater fish from the continental freshwater compartment	(109)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
IH_northseafish[continental]	continental daily intake of North Sea marine fish	0.000047	$kg_{wet\ marine\ fish} \cdot d^{-1}$
DOSE_northseafish[continental]	continental human dose through intake of marine fish from the North Sea	(110)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
IH_atlanticfish[continental]	continental daily intake of oceanic marine fish	0.01	$kg_{wet\ marine\ fish} \cdot d^{-1}$
DOSE_atlanticfish[continental]	continental human dose through intake of marine fish from the world oceans	(111)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
DOSE_leafcrops[continental]	continental human dose through intake of leaf crops	(112)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
DOSE_rootcrops[continental]	continental human dose through intake ofroot crops	(113)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
DOSE_meat[continental]	continental human dose through intake of meat	(114)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$

DOSE_dairy[continental]	continental human dose through intake of dairy	(115)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$
DOSE_totoral[continental]	continental total human oral dose	(116)	$kg_{chem} \cdot kg_{bw}^{-1} \cdot d^{-1}$

[2] Model outcome

DOSE_drw[regional] = C_drw[regional]*IH_drw/BW *(95)*

DOSE_freshfish[regional] = C_fish[regional]*IH_freshfish[regional]/BW (100)

DOSE_northseafish[regional] = C_seafish[northsea]*IH_northseafish[regional]/BW (101)

DOSE_atlanticfish[regional] = C_seafish[atlantic]*IH_atlanticfish[regional]/BW (102)

DOSE_leafcrops[regional] = C_leafcrops[regional]*IH_leafcrops/BW *(103)*

DOSE_rootcrops[regional] = C_rootcrops[regional]*IH_rootcrops/BW *(104)*

*DOSE_meat[regional] = C_meat[regional]*IH_meat/BW* (105)

*DOSE_dairy[regional] = C_dairy[regional]*IH_dairy/BW* (106)

DOSE_totoral[regional] =
DOSE_drw[regional]+DOSE_freshfish[regional]+DOSE_northseafish[regional]+DOSE_atlanticfish[regional]+DOSE_leafcrops[regional]+DOSE_rootcrops[regional]+DOSE_meat[regional]+DOSE_dairy[regional] (107)

DOSE_drw[continental] = C_drw[continental]*IH_drw/BW *(108)*

DOSE_freshfish[continental] = C_fish[continental]*IH_freshfish[continental]/BW (109)

DOSE_northseafish[continental] = C_seafish[northsea]*IH_northseafish[continental]/BW (110)

DOSE_atlanticfish[continental] = C_seafish[atlantic]*IH_atlanticfish[continental]/BW (111)

DOSE_leafcrops[continental] = C_leafcrops[continental]*IH_leafcrops/BW *(112)*

DOSE_rootcrops[continental] = C_rootcrops[continental]*IH_rootcrops/BW *(113)*

*DOSE_meat[continental] = C_meat[continental]*IH_meat/BW* (114)

*DOSE_dairy[continental] = C_dairy[continental]*IH_dairy/BW* (115)

DOSE_totoral[continental] =
DOSE_drw[continental]+DOSE_fish[continental]+DOSE_seafish[continental]+DOSE_freshfish[continental]+DOSE_northseafish[continental]+DOSE_atlanticfish[continental]+DOSE_leafcrops[continental]+DOSE_rootcrops[continental]
+DOSE_meat[continental]+DOSE_dairy[continental] (116)

PART II

TNO Environment, Energy and Process Innovation

Laan van Westenenk 501
Postbus 342
7300 AH Apeldoorn
The Netherlands

www.mep.tno.nl

T +31 55 549 34 93
F +31 55 541 98 37
info@mep.tno.nl

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Immobilisation of metals in North Sea and Ocean

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Authors C.C. Karman
K.I.E. Holthaus
R.G. Jak
R. Bernhard
K.J.M. Kramer*

* MERMAYDE, Bergen, NL

Order no. 32676

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1. Introduction

The REIM-SEA model was developed by CML (with input from TNO) as a tool for prioritising measures for reduction of emissions to the marine environment (Wegener Sleeswijk *et al.*, 1998), as was developed for air emissions some years ago (Kuyper, 1995). On the basis of LCA principles, emissions are weighed on their relative contribution to the total input of contaminants and the relative environmental impact. To determine these parameters, a multi-media model is used, estimating the distribution of contaminants over the various environmental compartments. Contaminants will disappear from the model system as a result of (bio-)degradation and, since only the water column is considered in the REIM-SEA model, by deposition to the sediment.

After performing test runs with the REIM-SEA model, metals (i.e., Cd, Cu, Ni, Pb, Zn, As and Hg) appeared to be weighed unrealistically high on the basis of their environmental impact. Further study revealed that the model, lacking a loss-term for metals, continuously accumulated metals, leading to increasingly high effects. In reality, however, metals are immobilised to a high degree by sedimentation or transported to the ocean and as such not available to cause biological effects in the North Sea.

In order to be able to include a better quantification for the loss of metals in the North Sea in the REIM-SEA model, this report will elaborate on the most important aspects with regard to immobilisation. An overview will be given of the forms (species) in which metals can be present in the water column (free ions, dissolved complexes and adsorbed to suspended material). Furthermore, the main flows of water and sediments (suspended material) through the North Sea will be described and quantified, in order to implement the deposition of metals bound to suspended matter as a loss term in the REIM-SEA model.

2. Fate and behaviour of metals in seawater

During the last decades a lot of work was put in the study of trace elements and trace metals in seawater. Aiming at an accurate prediction of metals in seawater it became clear that the measurement of concentrations should be linked to the measurement of metal species, i.e., the physical and chemical forms in which elements appear in seawater (Mackey and Zirino, 1994). Dissolved metals can form complexes with a wide range of (dissolved and particulate) organic and inorganic complexing agents, depending on pH, oxidation state and relative abundance of the complexing agents (Duinker *et al.*, 1974). It is this complexation (or adsorption in case of particulate matter) behaviour that determines the actual fate and behaviour - and thus immobilisation- of metals in seawater. Ultimately, the overriding justification for quantifying speciation is the fact that it is usually the free ion concentration of metals that leads to toxic effects. Although uptake with food (i.e., metals adsorbed to phytoplankton) may occur as well, this aspect is not considered relevant for explaining metal toxicity.

This chapter focuses on the main processes that remove metals from the fraction of free ions: adsorption to suspended material and complexation with dissolved compounds. Finally, some attention will be paid to the volatilisation of metals from the water column, which is unique for mercury.

2.1 Adsorption to suspended material

Interactions between particulates and metals play an important role in the 'regulation' of dissolved metal concentrations. Moreover, adsorption is the first step in the ultimate removal of trace metals from the hydrological cycle; the ultimate sink being the ocean sediments (Salomons and Förstner, 1984).

The distribution of constituents in estuaries and in shelf seas is dependent on the exchange of materials between particles and water. Especially physicochemical factors such as salinity, pH and Eh have a great influence on this exchange. Primary production also exerts influence on the distribution (van Hoogstraten and Nolting, 1991). The mineral nature of the suspended particulate matter is an important factor for the exchange of materials between particles and water. Certain minerals, such as clays, have a high adsorption capacity for a number of both organic and inorganic contaminants, whereas more silty and sandy fractions consist of inert minerals, which have a negligible adsorption capacity. This adsorption capacity/affinity strongly influences contaminant transport (OSPAR, 2000a).

A number of studies have shown that clay minerals, oxides, hydroxides, and sulphides not only act to remove metals from solution, but may also hold the metals in a manner that allows their later release back into the overlying water column. The

concentration and distribution of many elements (e.g. Ni, Cu, Zn, Cd) in sediments and overlying waters are strongly influenced by adsorption and/or coprecipitation with iron and manganese oxides. Consequently, it was suggested that the sediments could release significant quantities of metals back into the water column, depending upon metal partitioning and ambient conditions (Feijtel *et al.*, 1988). In relation to trace metal pollution in estuaries and biological availability, Hirst and Aston (1983) suggest, however, that the resuspension and oxidation of polluted anoxic sediments is not an important process because released (soluble) metals would directly be scavenged by the resuspended material.

The solid phases interacting with dissolved constituents in natural waters consist of a variety of components, including clay minerals and carbonates. These components are usually coated with oxides and organic substances. Organic surfaces for metal sorption could arise in three possible ways (Salomon and Förstner, 1984):

- From organisms such as bacteria and algae
- By the breakdown of plant and animal material
- From low molecular weight material sorbed onto substrates

The trace metal adsorption capacity of organic matter varies for the different metals. Figure 1 shows the half-life of metals in the water column as a function of the fraction of the total metal bound to particulate matter in a mesocosm study (DiToro *et al.*, 2001). Cd, Zn and Co have the lowest binding capacity to particulate matter and, as such, stay in the water column for a long time (half-life 25-40 days; Cd > 80 days). Mercury and chromate strongly adsorb to particulate matter and therefore have half-lives in the water column of 5 days and less. Table 1 shows comparable information for a large group of metals.

Delft Hydraulics (1999) studied the filtering capacity of estuaries (removal of contaminants by sedimentation of particles they adhered to). The capturing efficiency of the estuaries for the studied metals (Cd, Cu, Zn, Ni and Pb) was again in accordance with the binding capacity of the metals with particulate matter (lowest for Cd, highest for Pb).

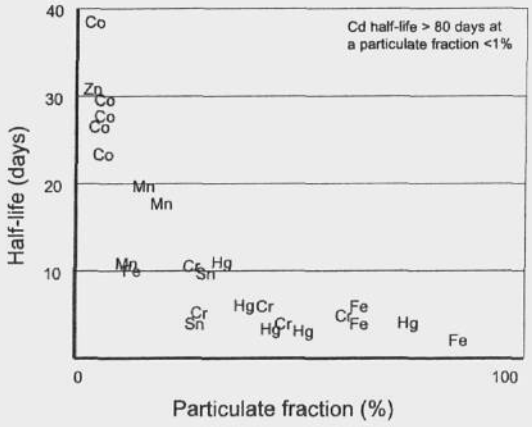


Figure 1. *Halflife of metals in the water column as a function of the fraction of metals bound to particulate matter (after: Di Toro et al., 2001).*

Table 1. *Grouping of metals on the basis of their half-life time in the water column of artificial test-systems (Santschi et al., 1982 in Salomon and Förstner, 1984).*

Classification	Metals	Half-live (days)	
		Winter	Summer
Particle reactive	Fe, Hg, Sn, Cr(III), Pb, Po, Th, Pa, Pu, Am, Be	10-20	2-3
Recyclable	Mn, Co	30-50	5-30
Biologically active	Zn, Cd, Se, As	60-100	10-50
Quasi conservative	Ba, Ra, Cs, Sb	150-600	80-150

2.2 Complexation

In surface waters, trace metals are present in a wide range of physicochemical forms both in the particulate and dissolved phases. The dissolved phase comprises the hydrated ions, inorganic and organic complexes, together with heterogeneous colloidal dispersions. These metals are often present in more than one valency state. The particulate phase also contains elements in a range of chemical associations, ranging from weak adsorption to binding in the mineral matrix. These species coexist although they may not necessarily be in thermodynamic equilibrium (Morrison *et al.*, 1989). Mackay and Zirino (1994) conclude that the speciation of trace metals in seawater is determined by a combination of kinetics and thermodynamics.

2.2.1 *Speciation chemistry*

In the aquatic environment, major and trace ions may react to form combinations, often through the process of complexation. If for example, a trace metal 'M' reacts with a trace anion (or ligand) 'L' we may have the reaction:

$$M + L \leftrightarrow ML \quad (1)$$

This reaction is rather simplified because the charges of the cation and anion are omitted. In addition, it identifies a two-directional reaction: formation of ML and dissociation to M and L (Stumm and Morgan, 1996). Nature strives to reach a state of equilibrium where the reactions involving complex formation (from left to right) and dissociation (reverse) are in balance.

The M can be a trace metal cation, like Cd^{2+}, Zn^{2+} or Cu^{2+}, or a major element like Ca^{2+} or Mg^{2+}, both abundant in seawater. The L, the ligand, may be Cl^-, $SO4^{2-}$, CO_3^{2-}, all inorganic in nature and abundantly available in seawater. The ligand can also be organic acids like amino, humic or fulvic. Various combinations between the large number of possible cations and anions are the basis of physico-chemical properties.

The position of the equilibrium does not usually lie in the middle where the concentration of reactants (M and L) equals the products (ML). While some complexation reactions have equilibrium that lie more towards the left (more free M and L present) most lie to the right (more ML complex is formed). The position of the equilibrium can be expressed as the ratio between the two sides of the reaction (1), defined as the stability or equilibrium constant K:

$$K = [ML] / [M] [L] \quad (2)$$

where the square brackets denote the concentrations of the complex ML, free M and free L, respectively (Stumm and Morgan, 1996). If the equilibrium constant is large, there is relatively more of the complex (reaction product) than when the K is small. Similarly, a large K results in a relatively small amount of the so-called 'free' metal (M^{2+}).

As each reactive metal can, in principle, react with each reactive anion, there are very large numbers of possible combinations in the aquatic environment. There exists a competition between the metals (e.g., Cu^{2+} and Pb^{2+}) for a given ligand (e.g., CO_3^{2-}). If the stability constant, K, for the $CuCO_3$ complex is higher than that for $PbCO_3$, than at equilibrium the complex with the highest K will be more abundant. Also other cations, trace metals as well as major ions (e.g. Ca^{2+}, Mg^{2+}, and hydrogen, H^+) will compete for the same carbonate. It becomes even more complex when we realise that there is not only one ligand L, but that there are numerous organic and inorganic ligands available in the aquatic environment. Many ligands

compete for the same element such as copper, but again, many ligands and many trace elements try to sort out the most energetically stable state: equilibrium.

2.2.2 The role of organic ligands

The effect of organic ligands upon the toxicity of trace metals has been recognised. Three decades ago, several researchers noted that in regions with upwelling waters the growth of phytoplankton was reduced. They attributed this effect to the lower content of organic ligands, and hence a reduction in the complexation of (free) copper (Steemann-Nielse and Wium-Andersen, 1971).

Many organisms, including bacteria, phytoplankton, macro-algae and snails, use the complexing potential of organic molecules as a detoxifying mechanism. This involves either ligands adsorbed to the outside of the organism (mainly with bacteria and phytoplankton) or ligands that are produced by the organism and excreted (exudates). This mechanism is a defence system against toxic trace metals. This defence system may be induced as function of the outside (ionic) trace metal concentration.

Fulvic and humic matter are another important group of organic ligands. They have demonstrated the ability to form complexes and subsequently cause a reduction in toxic effects (e.g. Giesy *et al.*, 1983; Winner, 1984; Florence *et al.*, 1992) Surface active organic compounds isolated from the marine environment have demonstrated a similar type of effect (Shine and Wallace, 1995).

2.2.3 Relative importance of speciation for a range of metals

When ranked, the relative importance of speciation (i.e., complex formation with ligands) decreases in the following order: Al > Cu > Co > Zn > Pb > Ni > Cd (Raspor *et al.*, 1984; Mackay and Zirino, 1994).

The dissolved fraction of copper, a highly reactive metal with respect to complex formation, exists in near-surface seawater primarily (usually to the extent of > 99%) as complexes with organic ligands. Copper complexation in the ocean is generally highest near the productivity maximum, and decreases by one to three orders of magnitude with depth below the vertical mixed layer (Sunda, 1988). Lead is divided between organic and inorganic forms, cadmium is mainly present as the free ion and zinc is present in both ionic and colloidal inorganic forms. (Allen *et al.*, 1980). Recent aniodic stripping voltametric measurements in central North Pacific surface water indicate that 98% of the zinc is complexed to relatively zinc-specific organic ligands (Sunda, 1988).

A generic quantification of the fraction of the total metals that is complexed with major organic and inorganic ligands cannot simply be given as complexation is, as described in paragraph 2.2.1., a highly complex process that is dependent on the

local situation at a specified time. However, Byrne *et al.*, (1988) have studied some generic relationships of the influence of temperature on pH and metal speciation in ocean waters. Some of their published data may be useful to derive a generic quantification, although its uncertainty must be noted.

2.3 Evaporation (Hg)

This last process that is described in this chapter on the fate and behaviour of metals is specific for mercury. In sea water, mercury ions can be converted into volatile mercury and emitted to the atmosphere. The resulting flux of mercury is estimated to be 4-10 t/yr in the North Sea, comparable to wet and dry deposition (OSPAR, 2000b).

3. Water and sediments transport

Independent of the exact form of the metal, it will be transported from its release side to other areas as a result of the water current. The final fat of the metals, however, varies between dissolved metals (either as free ion or in complexation) and metals adsorped to suspended material.

The most important transport pathways of water and sediment in the North Sea and the adjacent Atlantic Ocean will be described and, where possible, quantified in this chapter.

3.1 Water transport between the North Sea and Atlantic Ocean

A number of waterbodies can be distinguished in the North Sea on the basis of their origin and properties (salinity, temperature and the fluctuations of these parameters). Close to the Dutch coast, the water is continental and strongly influenced by the run-off of fresh water from rivers. Further to the west, saline Channel water is transported from south to north along the Dutch coastal areas, whilst Atlantic water is transported from the north (most relevant for the North Sea as a whole). The water of the Central North Sea is positioned between these water masses (Threlkeld and Choinsky 1985), and only slowly mixes with other watermasses.

The salinity and temperature characteristics of different areas are strongly influenced by heat exchange with the atmosphere and local freshwater supply. The deeper waters of the North Sea consist of relatively pure marine water and, in certain areas, is slightly modified through mixing with less saline surface water. The circulation and distribution of these water masses is of the utmost importance in supporting biological productivity, transport and concentration of living organisms (e.g. larvae) and non-living particulate matter in the region (OSPAR, 2000b).



Figure 2. Main water flows within, into and from the North Sea (OSPAR, 2000b).

The most relevant pathway of water transport is from the Northwest (Scotland) through the Southwest and Southeast of the North Sea to the North-East (Norway) where it flows out into the Ocean. A smaller flow of water comes in from the south (Channel) to join the above-described flow from the North (see Figure 2).

Some values for the residual flows of different water masses can be derived from recent studies of transport and long-term residual circulation in the North-West European shelf using hydrodynamic models (OSPAR, 2000b).

The latest model results for the years 1955-1998 indicate seasonal (1^{st}-4^{th} quarter) average transports of respectively: 1.5, 0.9, 1.1 and 1.4 10^6 m^3/s. These estimated outflows, that vary seasonally, are in close balance with similar estimates of all the inflows to the North Sea, including the rivers. The net seasonal average inflow through the Channel was modelled to be: 0.05, 0-0.01, 0.02 and 0.05 10^6 m^3/s for the same quarterly periods.

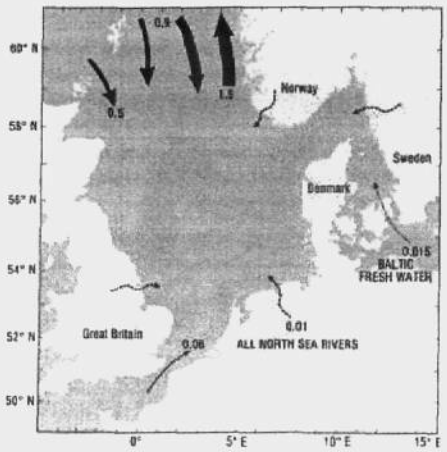


Figure 3. Modelled quantification of the waterflows (in 10^6 m^3/s) during wintertime into the Northsea and from the North Sea into the Atlantic Ocean (OSPAR, 2000b).

The residence time for the entire North Sea, including the Norwegian Trench, is estimated to be 1 year (OSPAR, 2000b). However, significant regional differences exist within the North Sea. The maximum residence time occurs in the central North Sea and is estimated to be approximately 3 years. Along the Dutch coast, however, residence times are much lower.

3.2 Sediment transport between the North Sea and Atlantic Ocean

Horizontal and vertical differences in densities of the saline North Sea water and the fresh water riverine inputs cause transverse circulation, resulting in high turbulence in the coastal zone. Also high wind speeds can stimulate the mixing of the water column. This results in coastward water current near to the bottom of the sea, leading to the erosion of large amounts of particulate organic material. This mechanism may also be present further away from the coast, unless the density gradients are strong enough to create an undercurrent (Klein and van Buuren, 1992).

The concentration of suspended material in the water column follows a seasonal cycle with a maximum in winter and a minimum in summer. The seasonal pattern in the concentration and the distribution of sediment particles is influenced by variable wind directions- and speeds, the activity of sources of suspended material (e.g. dead phytoplankton) and the amounts that are transported by the discharging rivers.

Figure 4 shows that erosion mainly occurs along the coast of Belgium, the Netherlands and Denmark, as well as in the central North Sea. This material is deposited in areas indicated as black grid cells (e.g., Oyster Grounds and Skagerrak).

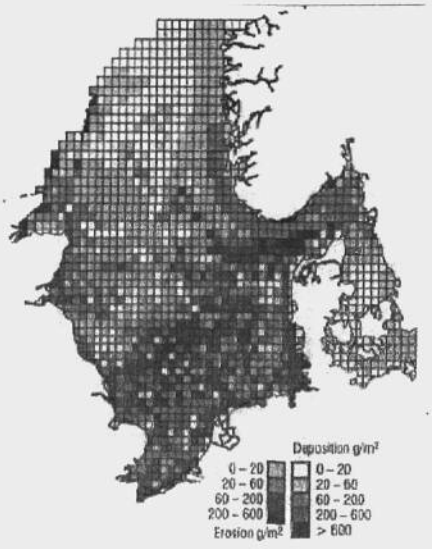


Figure 4. *Areas of erosion and deposition in the North Sea. In red areas there is a net erosion, while the black areas are actual deposition areas (OSPAR, 2000b).*

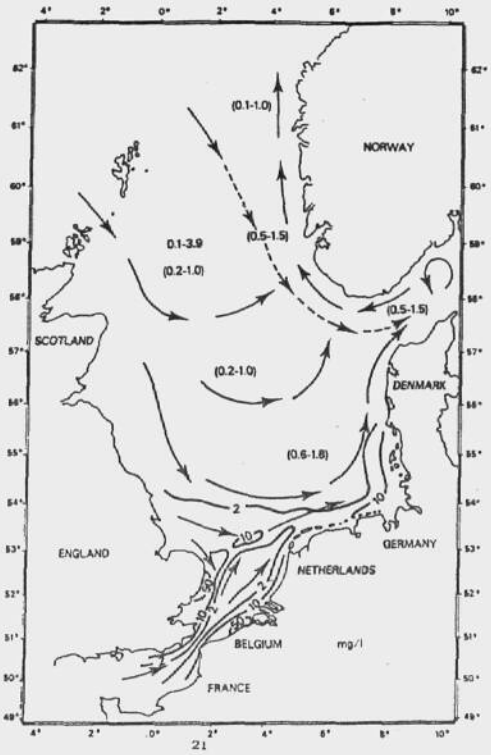


Figure 5. Main transport routes of sediment within the North Sea (Delft Hydraulics Laboratory, 1983).

The concentration of suspended matter in the surface water of the Atlantic Ocean is very low, while on the continental shelves it is generally higher. In the North Sea the winter concentration generally increases from north to south and from offshore to inshore. The reason that the suspended matter concentration of oceanic surface waters is so much lower than of water on the shelf is that there are no nearby sources, such as rivers and a shallow seafloor, where resuspension may occur, whereas the particulate matter produced by phytoplankton sinks out from the surface layer.

The suspended matter concentration is much higher in the oceanic water that enters the southern North Sea through the Dover Straits than in the Atlantic water at the northern boundary. Most of this material is picked up from the Channel coasts and seafloor and therefore is not of oceanic origin. Thus, although the water inflow from the south is relatively small, the input of particulate matter is higher than from the northern boundary. The concentration of suspended matter flowing in and out

at the northern boundary between Scotland and Norway is approximately the same and taking into account the small excess of the water outflow over the inflow this implicates that only a little more suspended material is exported than imported (Table 2).

Table 2. Input, output and bottom deposition of suspended material in the North Sea predicted from models (OSPAR, 2000b)

	10^6 t/yr
Input	
North Atlantic ocean	10.4
Channel	22-30
Baltic	0.5
Rivers	4.8
Seafloor erosion	approx. 9-13.5
Coastal erosion	2.2
Atmosphere	1.6
Primary production	1
Total input	*51.5-64*
Output	Approx. 11.4-14.3
Deposition	
Estuaries	1.8
Wadden Sea and The Wash	5
Outer Silver Pit	approx. 1-4
Elbe Rinne	?
Oyster ground	approx. 2
German Bight	3-7.5
Kattegat	8
Skagerrak and Norwegian Trench	approx. 17
Dumped on land	2.7
Total deposition	approx. 51 (51.9-62.4)

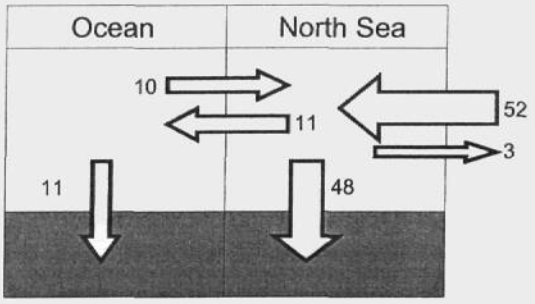


Figure 6. Schematic presentation of the mass balance of suspended material transports in the North Sea in relation to the Atlantic Ocean (in 10^6 tons/yr).

3.3 Residence times of metals in the North Sea and Atlantic Ocean

3.3.1 North Sea

The North Sea system is largely different from the situation in the oceans. This is due to the bathymetry of the system, the currents regime and hydraulic residence times (for different water bodies), the importance of inputs in the area (also atmospheric), suspended particulate matter content (also due to resuspension), the high biological activity.

Concentrations, both dissolved and particulate are found to be highest in the coastal zones, the areas with the highest (riverine) inputs (e.g. Kremling, 1983; 1985; Balls, 1985; Danielsson *et al*, 1985; Nolting and Eisma, 1988; Kramer *et al.*, 1991; Kersten *et al.*, 1991; Hydes and Kremling, 1993; Haarich and Schmidt, 1993; Laslett, 1995; Scholten *et al.*, 1998; OSPAR, 2000a).

There is, however, still a difference between northern North Sea and open Atlantic Ocean waters. A slight increase (x2) has been observed when travelling across the shelf edge, notably for Cu, Cd and Ni (Kremling, 1983; 1985; Balls, 1985; Kremling and Hydes, 1988). For biogenic elements (Cd, Zn, Cu, Ni, As) there may be an effective trapping at the shelf edge, especially in summer. Nutrient rich inflow water sustains primary production, with resulting uptake of these elements by phytoplankton (particulate phase).

Due to the SPM concentration, and the size spectrum of North Sea suspended matter, scavenging by particles is important; but due to the water depth, supply from sediments, where diagenetic processes recycle trace elements, is evident (Burton *et al.*, 1993). In contrast to the oceans, sedimentation not necessarily leads to output of the system. In large parts of the North Sea resuspension of particles takes place, which may be the result of tidal currents, storm induced turbulence and benthic fisheries. Only in the deeper areas, such as the Skagerrak and Norwegian Trench, net sedimentation occurs. Despite this it is generally assumed that most particulate material remains in the North Sea area. Only a small fraction (fine) SPM will escape to the open Atlantic. This is supported by the observation that particulate concentrations in in- and outflow are very similar.

Water transport (which is the carrier for all dissolved and non-depositing particulate components) in the North Sea is difficult to estimate. Not only are there large seasonal and inter annual differences in inflow (mainly as a result of changes in the North Atlantic Oscillation: NAO), also different areas in the North Sea show different values for water mass transport and consequently flushing times (hydraulic residence times). Laane *et al.* (1996) showed – using nutrient data - that variations due to the NAO in North Atlantic inflow have far reaching consequences for the transport of (dissolved) components. In paragraph 3.1 some modelling studies in attempt to model this water transport are described.

For the entire North Sea flushing times are estimated 350-500 days. Care has to be taken when interpreting such data. For example, in the Skagerrak the flushing time of the surface waters is in the order of months, for the deep water it is in the order of years. Calculated regional differences (sub-regions) are presented in OSPAR (2000a) provides flushing times for the various sub-regions of the North Sea.

As a result of this complex mixture of interacting processes, as far as known to the author, no residence times have been calculated for trace elements in the North Sea. Sündermann (1994) contains concepts of approaches, but no actual data.

3.3.2 Atlantic Ocean

The residence time of an element in the oceans is the average time it is present in the sea before being removed into the sediment sink (or escapes to the atmosphere). In a steady state (!) system it is assumed that the input is balanced by the output. Often the following expression is used to calculate the residence time (τ):

$$\tau = A / (dA/dt)$$

where A is the total amount of the element (particulate + dissolved), and) dA/dt the amount introduced or removed per unit time. Such an approach requires that the element is completely mixed in the system in a time that is short in comparison to the residence time, and that neither A nor dA/dt change appreciably in 3-4 times this period (Chester, 1990).

Usually the inputs are simplified by defining that rivers enter into the oceans directly, without taking into account estuarine and/or shelf sea processes (retention). Bewers and Yeats (1977) therefore used net river inputs. The mean oceanic residence time (MORT) concept was developed by Whitfield (1979), defined as the total quantity of an element present in the oceans divided by its input rate (from rivers) or its output rate (sedimentation).

The calculation of residence times is becoming much more complex if the hydrography, element-particle interactions and element-biota interactions are taken into account. Wangerski (1986) postulated that as a consequence surface water residence times are not constant on an ocean scale. The above mentioned concept $\tau = A / (dA/dt)$ seems to work well for conservative elements (Na, K, Mg, ...). Non-conservative elements are more complex. Dissolved elements that undergo passive particle scavenging (sorption, surface complexation) tend to have relatively short residence times with respect to the mixing time of the oceans. Particle association and subsequent deposition will lower the residence time considerably. In addition, nutrient-type elements that are involved in an active biological removal mechanism, undergo a surface water depletion and sub-surface regeneration. These elements take part in upwelling, biological uptake, vertical transport via particulate organic carriers, and regeneration at depth. This may result in repeated internal cy-

cles for these nutrient-type elements (including Cd, Cu, Ni, Zn, As) before their final removal in the sediments. It will be long relative to the mixing cycle of the oceans (about 1,600 y).

In Table 3 an overview is presented of (oceanic) residence times for the elements Cd, Cu, Ni, Pb, Zn, Hg and As. No residence times have been found in the literature that focus on the surface layer only.

Table 3 Characteristics and residence times of trace metals in seawater

	Cd	Cu	Ni	Pb	Zn	Hg	As	Reference
Concentration (nmol/kg)								
world ocean, range (S=35)	0.001-1.1	0.5-6	2-12	0.005-0.175	0.05-9	0.002-0.01	15-25	Bruland, 1983
world ocean average	0.7	4	8	0.01	6	0.005	23	Bruland, 1983
Type	nutrient	nutrient & scavenging	nutrient	high surface depleted at depth	nutrient	??	nutrient	Bruland, 1983
ocean residence time (in y)								
	5 x 10^5	4.3 x 10^4	1.5 x 10^4	5.6 x 10^2	1.8x10^5	4.2x10^4	-	Goldberg, 1965
	-	5 x 10^4	1.8 x 10^4	2 x 10^3	-	-	-	Goldberg, 1965
	-	2 x 10^4	9 x 10^4	4 x 10^2	2 x 10^4	8 x 10^4	5 x 10^4	Brewer, 1975
	7.7-92 x 10^3	4.1-6.4 x 10^4	1.8-3.6 x 10^3	-	0.78-1.8 x 10^4	-	-	Bewers & Yeats, 1977
	-	9.7 x 10^2	8.2 x 10^3	8.1 x 10^1	5.1 x 10^2	5.6 x 10^2	3.9 x 10^4	Broecker & Peng, 1982
	-	-	6 x 10^3	-	-	-	-	Martin & Whitfield, 1983
	1.8 x 10^4	2.4 x 10^3	1.4 x 10^4	1.1 x 10^3	1.2 x 10^2	1.8 x 10^4	3.2 x 10^4	MORT, Martin & Whitfield, 1983
	-	5 x 10^3	-	-	-	3.5 x 10^2	-	Gill & Fitzgerald, 1988

4. Immobilisation of metals in the North Sea and Ocean

This report aims at providing insight in the processes that form the basis of the immobilisation of metals in the North Sea and Atlantic Ocean. The role of adsorption and speciation has been described, as well as the transport of water and suspended material in the North Sea and the exchange with the Atlantic Ocean. The combination of these two processes forms the key to immobilisation.

The toxicity of metals is mainly related to the bioavailable dissolved ionic fraction. From the total amount of metals present in seawater, only a small percentage appears in a dissolved form. Dissolved metals form complexes with inorganic and organic ligands, and further reduce the bioavailability of metals. A substantial part (up to 90% or higher) of the metals is bound to particulate matter, including sediments.

The North Sea is flushed with water from the ocean, with an average residence time of approximately 1-2 years. This effectively means that metals present in dissolved form (either complexed or in free ionic form) may be transported out of the North Sea within one year. As mentioned above, however, dissolved metal concentrations are insignificant in comparison to metals bound to suspended matter (both organic and inorganic). The majority of the suspended matter is deposited in the North Sea, while the remainder is transported to the ocean where it will be deposited. It can therefore be concluded that the seabed (where suspended sediments are deposited) acts as a trap for metals and most metals do not leave the North Sea area. Actual residence times for metals in the North Sea have never been estimated.

When subsequent adsorption to suspended material and deposition on the seabed is considered the most significant process of immobilisation, up to 90% of the metals present in the water column may be immobilised and not be bioavailable for causing environmental effects (as the remaining dissolved fraction forms immobile complexes which further reduces bioavailability, this still may be considered a worst case assumption). The capacity of individual metals to adsorb to suspended material, however, shows a large variation. No residence times of metals in the North Sea are available, a classification of the adsorption to suspended material (which is a key factor in the bioavailability of metals) can be made on the basis of the half-life time in the watercolumn (see also paragraph 2.1):

- High immobilisation: Cu, Hg, Pb (half-life time 10-20 days)
- Lower immobilisation: Zn, Cd, As, Ni (half-life time 60-100 days)

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6. Authentication

Name and address of the principal:
NOGEPA
C.W. van Oosterom
Postbus 11729
2502 AS Den Haag

Names and functions of the cooperators:

K.I.E. Holthaus	Project leader
C.C. Karman	Research scientist
R.G. Jak	Research scientist
R. Bernhard	Research scientist

Names and establishments to which part of the research was put out to contract:
K.J.M. Kramer, Mermayde, Bergen, NL

Date upon which, or period in which, the research took place:
2001

Signature: Approved by:

K.I.E. Holthaus
Project leader
April 12, 2002

C.C. Karman
Head of Department
April 12, 2002