RIVM report 601501027/2005

Environmental Risk Limits for alcohols, glycols, and some other relatively soluble and/or volatile compounds

2. Integration of human and ecotoxicological risk limits

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This investigation has been performed for the account of the Directorate-General for Environmental Protection, Directorate for Chemicals, Waste and Radiation, in the context of the project 'International and National Environmental Quality Standards for Substances in the Netherlands', RIVM-project no. 601501.

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Rapport in het kort

Milieurisicogrenzen voor alcoholen, glycolen en enkele andere relatief oplosbare of vluchtige stoffen. 2. Integratie van risicogrenzen voor mens en ecosystemen

Milieurisicogrenzen zijn concentraties van een stof in water, bodem, sediment en lucht waarbij geen nadelige effecten van die stof worden verwacht. In dit rapport worden milieurisicogrenzen bepaald die zowel de mens als ecosystemen beschermen tegen nadelige effecten van chemische stoffen. Hiertoe werden eerder afgeleide ecotoxicologische risicogrenzen vergeleken met die voor de mens: 1-butanol, *n*-butylacetaat, cyclohexylamine, diethyleenglycol, ethyleenglycol, ethylacetaat, methanol, methyl ethyl keton (MEK), methyl *tert*-butyl ether (MTBE), tribroommethaan en triethanolamine.

De milieurisicogrenzen voor de mens die in dit rapport zijn gerapporteerd zijn berekend met behulp van het model Humanex. Humanex is beschreven in RIVM rapport 601501022. De milieurisicogrenzen op basis van de ecotoxicologie zijn berekend in deel 1 van dit rapport (RIVM rapport 601501016). De hier gepresenteerde methode maakt het mogelijk om relatief eenvoudig uit te rekenen of humane risico's dominant zijn over het milieu of andersom. Voor 4 tot 5 stoffen (afhankelijk van het milieucompartiment) blijkt de mens de meest kritische factor te zijn voor het risico van de stof.

Trefwoorden: geïntegreerde risicoschatting; mens; milieu, blootstelling; model; chemische stoffen; normstelling, risicogrenzen

Abstract

Environmental Risk Limits for Alcohols, Glycols, and other Relatively Soluble and/or Volatile Compounds. 2. Integration of Human and Ecotoxicological Risk Limits

Environmental risk limits are concentrations of a substance in water, air, sediment and soil that are expected to be protective of the environment. In this report environmental risk limits (ERLs) are derived, based on a comparison of human and ecotoxicological risk limits. Ecotoxicological risk limits, derived previously, were compared to risk limits for human health for the following substances: 1-butanol, *n*-butyl acetate, cyclohexylamine, diethylene glycol, ethylene glycol, ethyl acetate, methanol, methyl ethyl ketone (MEK), methyl *tert*-butyl ether (MTBE), tribromomethane and triethanolamine.

Environmental risk limits based on ectoxicological information were calculated in part 1 of this report (RIVM report 601501016). The scientific basis for the human risk evaluation model Humanex is described in a companion report (RIVM report 601501022). The method presented here allows a relatively easy calculation of the dominant risk to either humans or to the environment. Human risk appeared to determine the risk limits for four to five substances (depending on the environmental compartment).

Keywords: integrated risk assessment, environment, health; exposure; model; chemicals; quality objectives

Contents

Samenvatting

Milieurisicogrenzen moeten bescherming bieden aan mens aan milieu. Bij het afleiden van milieurisicogrenzen in het kader van interventiewaarden worden deze grenzen afgeleid voor zowel de mens en het milieu, waarna de laagste waarde wordt voorgesteld als milieukwaliteitsnorm. Bij het afleiden van milieugrenzen voor de algemene milieukwaliteit werd tot nu toe alleen voor een aantal vluchtige stoffen gekeken naar het risico voor de mens. In voorgaande rapporten werd echter vastgesteld, dat het voor deze stoffen niet uitgesloten is, dat blootstelling ook via andere routes dan alleen lucht plaatsvindt. Op basis hiervan heeft de voormalige Stuurgroep INS (thans Stuurgroep Stoffen) vastgesteld dat een multi-compartimentele benadering van humane blootstelling het meeste perspectief biedt. Het rapport geeft een invulling aan deze benadering,

In dit rapport zijn maximum toelaatbare risiconiveaus vergeleken voor 11 stoffen waarvoor risico's voor mens en milieu worden verwacht: 1-butanol, *n*-butylacetaat, cyclohexylamine, diethyleenglycol, ethyleenglycol, ethylacetaat, methanol, methyl ethyl keton (MEK), methyl *tert*-butyl ether (MTBE), tribroommethaan (bromoform) en triethanolamine. Risicogrenzen voor het milieu zijn eerder berekend op basis van toxiciteitsgegevens voor deze stoffen met verschillende organismen. De risico's voor de mens werden berekend met het model Humanex. Dit model berekent het relatieve belang van blootstellingroutes naar de mens, op basis van de fysisch-chemische eigenschappen en de emissies tijdens productie en gebruik. Hiermee kan berekend worden, wat de concentraties in de verschillende milieucompartimenten mogen zijn, waarbij de totale blootstelling van de mens de toelaatbare dagelijkse inname (TDI) net niet overschrijdt.

Uit de vergelijking van de risicogrenzen voor mens en milieu kwam naar voren dat de mens de meest kritische factor is voor milieurisicogrenzen voor 4 tot 5 stoffen, afhankelijk van het milieucompartiment. In die gevallen kan de risicogrens voor een bepaald milieucompartiment naar beneden worden bijgesteld, zodat er geen risico voor de mens is. Op theoretische gronden is dit een goede keus. Binnen het kader van het project '(Inter)nationale Normstelling Stoffen' (INS), wordt de methodologie van het 'Technical Guidance Document' (TGD), uitgebracht door de Europese Commissie, gebruikt. In deze richtlijn wordt altijd een integratie van humane en ecotoxicologische risico's gemaakt. Deze bijstelling is echter misschien niet altijd nodig. Er zijn redenen om alleen de risicogrens naar beneden bij te stellen, als het betreffende compartiment daadwerkelijk een belangrijke bron is van blootstelling. Het gebruikte model laat zien of dit het geval is of niet, en in welke mate. Het hier gepresenteerde model maakt het eenvoudig om de bepalende factor, voor milieurisicogrenzen te vinden: mens of milieu. Zonder modelberekeningen is dit niet in te schatten.

Summary

Environmental risk limits should offer protection to man and ecosystems. Risk limits in the framework of soil remediation (so called intervention values) are derived in that way. The strictest limit is proposed as official quality standard. In the framework of general environmental quality, the maximum permissible concentration only took human risk into account for a number of volatile substances. Previous research however showed that for these substances, it could not be excluded that other routes of exposure could contribute to human risk as well. On that basis, the steering committee (currently Steering Committee for Substances) for this project (INS) decided that a multi-route approach to human exposure is more appropriate. This report details such an approach.

In this report, maximum permissible concentrations (MPCs) were compared for eleven substances for which risks to both man and environment are expected: 1-butanol, *n*-butyl acetate, cyclohexylamine, diethylene glycol, ethylene glycol, ethyl acetate, methanol, methyl ethyl ketone, methyl *tert*-butyl ether, tribromomethane and triethanolamine. Ecotoxicological risk limits were calculated in a companion report, based on laboratory toxicity tests with several organisms. Risks for man were calculated with the model Humanex. This model calculates the relative importance of exposure routes to man, based on the phyico-chemical properties of a substance and the emissions that take place during production and use of a substance. This allows for estimation of concentrations in each environmental compartment, where total human exposure is just within the limits of the tolerable daily intake (TDI).

The comparison between ecotoxicological and human risk limits showed that human risk was the critical factor that determined risk limits for four to five substances (depending on the compartment). In those cases, the risk limits can be adjusted downwards such that no risk to humans remains. This is a good choice on theoretical grounds. Within the framework of the project ‘International and National Environmental Quality Standards for Substances in the Netherlands’, the methodology from the Technical Guidance Document (TGD), issued by the European Commission, is used. In this guidance an integration of human and ecotoxicological risks is always made. However, this adjustment may not always be needed. It can also be argued that risk limits are only adjusted downwards, if that particular compartment is an important exposure route for humans. The model that was used can identify if this is the case and to what extent. The model presented here makes it easy to determine the critical factor that determines the risk limits: man or environment. It is not possible to do this without model calculations.

1. Introduction

1.1 General background

This report is a result of the project 'International and National Environmental Quality Standards for Substances in the Netherlands'. The aim of the project is to derive environmental risk limits (ERLs) for substances in the environment for the compartments air, (ground)water, sediment and soil. This specific report focuses on the integration of risk limits for man and ecosystems. The strictest criterion is used to determine the final risk limit.

ERLs serve as advisory values to set environmental quality standards (EQS) by the Steering Committee for Substances for various policy purposes. The term EQS is used to designate all legally and non-legally binding standards that are used in Dutch environmental policy and Table 1 shows the correspondence between ERLs and EQSs. The general procedure for deriving ERLs is described in Traas (2001) and Janssen *et al*. (2004). The various ERLs are:

- the negligible concentration (NC) for water, soil, groundwater, sediment and air
- the maximum permissible concentration (MPC) for water, soil, groundwater, sediment and air
- the ecotoxicological serious risk concentration (SRC_{eco}) for water, soil, groundwater and sediment

Table 1. Environmental risk limits (ERLs) and the related environmental quality standards (EQS) that are set by the Dutch government in the Netherlands for the protection of ecosystems.

Description	ERL	EQS
The NC represents a value causing negligible effects to ecosystems. The NC is derived from the MPC by dividing it by 100. This factor is applied to take into account possible combined effects.	NC (for air, water, soil, groundwater and sediment)	Target value (for air, water, soil, groundwater and sediment)
The MPC is the concentration of a substance in air, water, soil or sediment that should protect all species in ecosystems from adverse effects of that substance. A cut-off value is set at the fifth percentile if a species sensitivity distribution of NOECs is used. This is the hazardous concentration for 5% of the species, the $HC5_{NOEC}$.	MPC (for air, water, soil, groundwater and sediment)	MPC (for air, water and sediment)
The SRC_{eco} is the concentration of a substance in the soil, sediment or groundwater at which functions in these compartments will be seriously affected or are threatened to be negatively affected. This is assumed to occur when 50% of the species and/or 50% of the microbial and enzymatic processes are possibly affected, the $HC50_{NOEC}$.	SRC_{eco} (for water, soil, groundwater and sediment)	Intervention value after comparison with SRC_{human} (for soil, sediment and groundwater)

The process of deriving ERLs is shown schematically in Figure 1. ERLs for soil and sediment are calculated for a standardized soil. ERLs for water are reported for dissolved and total concentrations (including a standard amount of suspended matter) and if found significantly different, differentiated to freshwater and saltwater. Each of the ERLs and its corresponding EQS represents a different level of protection, with increasing numerical values in the order of

Target Value < MPC[1] < Intervention Value. Each EQS demands a different action when exceeded, as explained elsewhere (VROM, 1994).

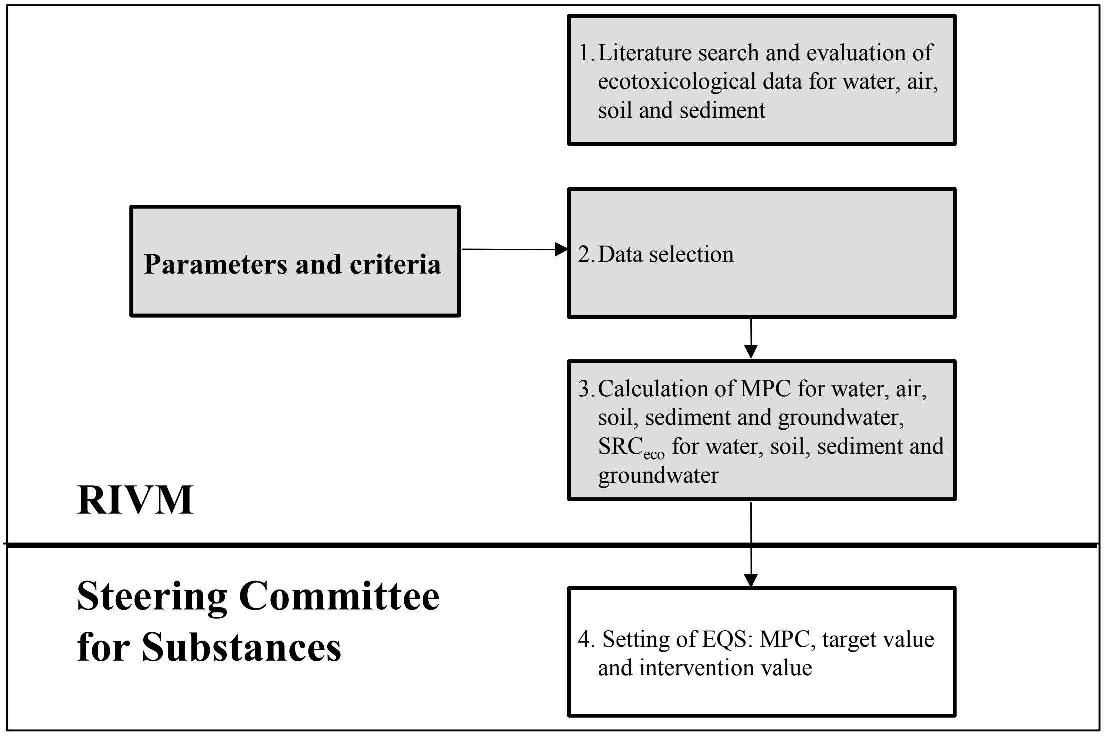

Figure 1. The process of deriving Environmental Risk Limits. Above the line the method to derive ERLs is indicated, i.e. MPC, NC and SRC_{eco}. *Below the dashed line the MPC, Target Value and Intervention Value is indicated, set by the Steering Committee for Substances.*

1.2 Human risk limits

People can be exposed to substances in soil, air, water or food products. Environmental quality standards are a policy instrument to safeguard against adverse effects of substances. In the Netherlands, the environmental risk limit ‘maximum permissible concentration (MPC)’ should protect both man and ecosystems. This report documents how the human exposure model ‘Humanex’ (Bontje *et al.*, 2005) was used to calculate MPCs for humans and how these are compared to MPCs for ecosystems.

In the past, a human risk characterisation was done for volatile substances where a suspicion existed that human risk could be dominant over ecotoxicological risk (Van de Plassche and Bockting, 1993). For volatile substances it is often assumed that inhalation through air is the predominant route of exposure for man. A previous study has shown that this is not always true (Mennes *et al.*, 1995). Calculating human exposure only from air causes an underestimation of the exposure. When more routes are added, the total exposure will increase.
In 1995 the Committee on integrated environmental quality objectives (‘Stuurgroep Integrale Normstelling Stoffen’) concluded that multiple routes of exposure should be taken into account when calculating MPCs, so no relevant route of exposure would be ignored. The

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[1] A complicating factor is that the term MPC is used both as an ERL and as an EQS. For historical reasons, however, the same abbreviation is used.

committee also confirmed that it was necessary to take the partitioning of substances into account when setting maximum permissible concentrations (MPCs) for water, sediment, soil and air (Gezondheidsraad, 1995). This partitioning of substances is implemented by the use of multi-media exposure models (Mackay, 1991). Multi-media models are used to predict concentrations of substances in the environment.

Currently, human risk limits are integrated with ecotoxicological risk limits in two ways:

1) Intervention Values for contaminated soil, sediment and ground water are based on a comparison of risk limits for man and ecosystems. The Intervention Values (concentrations) in environmental compartments are based on a calculation from a maximum permissible intake level (MPC_{human}) and are calculated with the model CSOIL (Van den Berg and Roels, 1995). The final risk limits are determined by the most critical target, man or ecosystems.
2) In the project 'International and National Environmental Quality Standards for Substances in the Netherlands' (INS), risk assessment for humans has only been done for a large group of relatively volatile substances (Van de Plassche and Bockting, 1993). To compare human and ecotoxicological risk limits, the concentration in air was calculated with the multi-media modeSimpleBox (Van de Meent, 1993). The assumption was that air concentrations are in steady-state with the available ecotoxicological risk limits for soil and water. The air concentration that is in steady-state with the ecotoxicological risk limits, is compared to a human-toxicicological risk limit for inhalation. If the tolerable concentration in air (TCA) is exceeded, the risk limit for air should be adjusted downwards (Van de Plassche and Bockting, 1993; Mennes *et al*., 1998).

There is a difference in approach between the two frameworks. In the framework of soil remediation, the risk of humans of living on contaminated soil is described by a specific scenario. It takes into account that people are exposed to the soil by way of soil contact, breathing in air that evaporates from the soil, and some part of the diet (vegetables and root crops) is home-grown on contaminated soil. This scenario is significantly different from the one that is used in the context of INS. In the latter framework, the risk is not due to living on contaminated soil, but on chronic, diffuse background exposure to the total of most relevant exposure routes. Because of the potential of substances to partition over different environmental phases, this exposure can be by way of food, drinking water, air, soil contact etc. The basic assumption behind this calculation, as implemented in EUSES, is that all compartments are in steady-state at a low, background level, and that the contaminant can reside in every compartment that is a potential route of exposure. In the EU framework for risk assessment of new and existing substances, this is referred to as 'indirect human exposure', as opposed to direct exposure e.g. in the workplace. This report documents the current method to calculate human risk limits for (background) multi-route exposure from a contaminated environment.

1.3 Exposure models

Contaminants may accumulate in the environment and eventually enter the human food chain. To assess the exposure of a person through food one has to actually measure the concentration of the contaminant for every single item of food and measure total food intake. This is not feasible for the purpose of general risk assessment; therefore more generic human exposure models have been developed.

To make an exposure assessment, estimates are used for an average person. To estimate parameters such as average body weight and other biophysical parameters statistics are used.

The European Union has developed the computer program EUSES (European Union System for the Evaluation of Substances) to assess the exposure of Europeans to contaminants in the environment (Lijzen and Rikken, 2004).

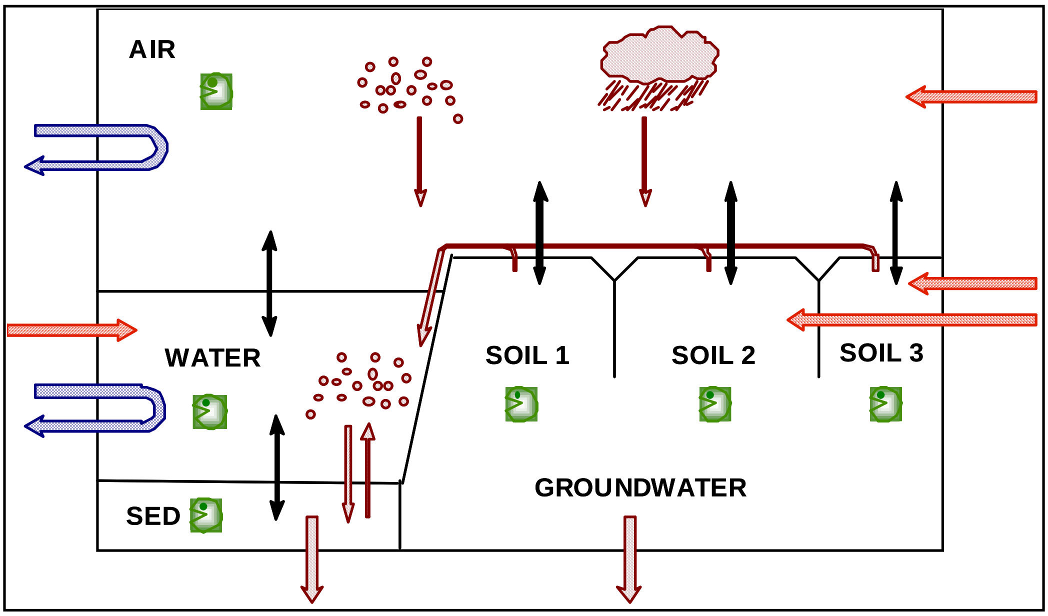


Figure 2. Environmental compartments considered in EUSES (EC, 1996).

The exposure to a given compound can be calculated. When actual measurements of the concentrations in the compartments such as air, water and soil are lacking, EUSES will use production volumes, compound properties and emission estimates to calculate likely concentrations in the environment. The predicted environmental concentrations (PECs) are then used to calculate the exposure of humans from air, drinking water, meat, milk, fish and crops.

To estimate the exposure of a person living on a polluted site, a risk assessment needs to be performed. Several human exposure models have been developed that often serve different goals. For an overview, see Swartjes (2002). In the Netherlands, the CSOIL-model was developed to estimate the exposure of humans who live on contaminated soil. This model includes routes not present in EUSES: exposure from home grown crops, soil ingestion, dust inhalation, dermal exposure to dust, inhalation of contaminants, evaporated from the soil or ground water, permeation of contaminants from the pore water into the drinking water and the exposure from showering with polluted drinking water.

By combining the CSOIL and EUSES model a comprehensive model has been built to describe multi-media exposure. Existing literature on this issue has been taken into account (Rikken *et al*., 2001; Rikken en Lijzen, 2004). This multi-media exposure model calculates human exposure and is named INS-Humanex. A companion report gives full details on the Humanex model and how it relates to both EUSES and CSOIL (Bontje *et al*., 2005).

Table 2 and Figure 3 show the exposure routes incorporated in Humanex. Consumption patterns in Humanex are based on the average diet in the Netherlands, instead of the average European diet as incorporated in EUSES (Bontje *et al*., 2005).

1.4 Integration of environmental risk limits

Ecotoxicological risk limits for several compounds were derived in previous reports (Verbruggen *et al.*, 2005; Tables 1-4; EU-RAR (EC, 2002) for MTBE). Results from this study will be used in the comparison between risk limits for human and ecological endpoints. Environmental concentrations related to human risk of these substances is calculated using the Humanex model as described above.

Table 2. Routes of exposure in the Humanex model, compared to EUSES and CSOIL.

EUSES-model	CSOIL-model	Humanex-model
Air	n.i.	Air
n.i.	Inhalation of contaminant evaporated from the soil Differentiation between inside and outside air.	Equal to outside air No differentiation
Meat[1]	n.i.	Meat
Milk[2]	n.i.	Milk
Fish	n.i.	Fish
Crops: root, leaf	Home grown crops: root, leaf	Crops: root, leaf
Drinking water purification	n.i.	Drinking water purification
n.i.	Permeation of contaminant from the soil into the drinking water	Permeation of contaminant from the soil into the drinking water
n.i.	Showering with drinking water	Showering with drinking water
n.i.	Soil ingestion	Soil ingestion
n.i.	Dust inhalation	Dust inhalation
n.i.	Dermal exposure to dust	Dermal exposure to dust

n.i. = not implemented, [1] Meat = all meat sources, [2] Milk = all dairy products

Human risk calculations starts from predicted regional environmental concentrations (PECs) calculated in EUSES. The compartments considered in EUSES are shown in Figure 1.3.

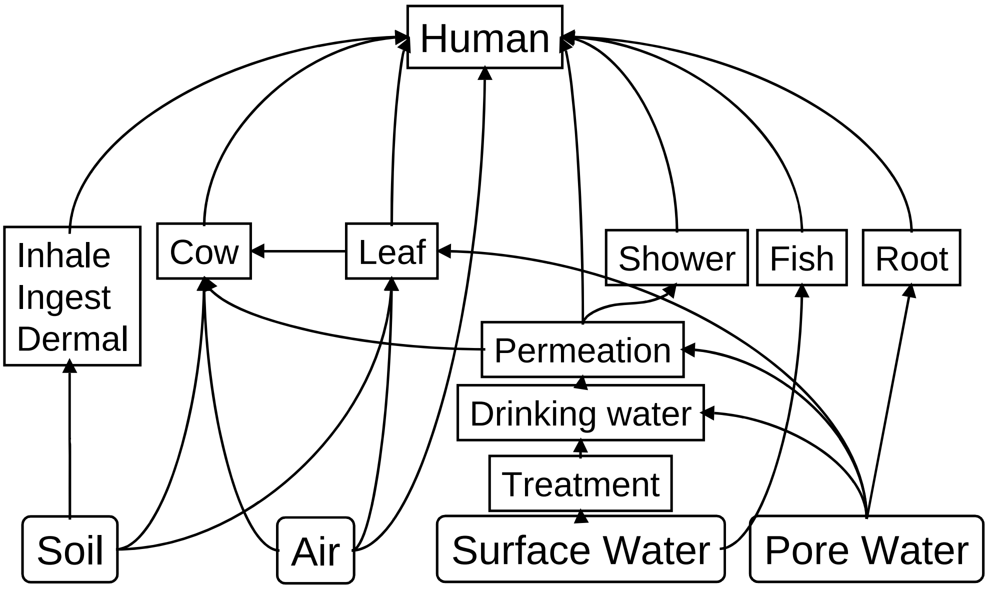


Figure 3. All routes of exposure in the Humanex model. Cattle includes meat and milk.

To calculate PECs, physico-chemical properties of substances and production information (industry and use category) are needed as input in EUSES.

The PECs, substance properties, and data about human exposure are combined into a set of equations in the Humanex model (Bontje *et al*., 2005). Humanex calculates contaminant concentration *ratios* in e.g. fish, cows, drinking water, air, crops and dust. These contaminant concentration *ratios* in human exposure media are subsequently used to calculate exposure *ratios* for direct and indirect human exposure (Figure 3), and the corresponding concentrations in the environmental media (water, air, soil, sediment). The human risk limits are compared to ecotoxicological risk limits, based on the concentrations in each environmental compartment (Figure 4).

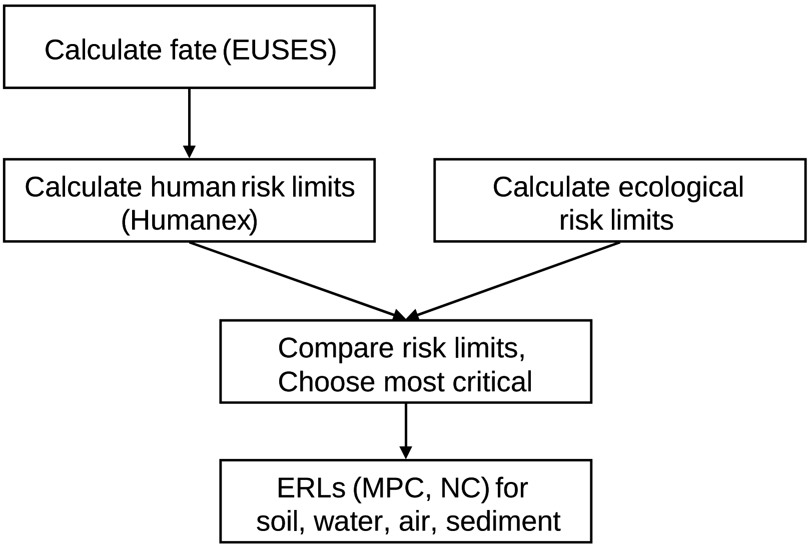


Figure 4. Diagram of the derivation of environmental risk limits (ERLs), based on integration of human and ecological risk.

A comparison of both types of risk limits will indicate the most sensitive target (humans or ecosytems) that will determine the final risk limit in each compartment. The compounds studied are shown in Table 3. These compounds have been choosen because of there physical-chemical properties which suggest relevant human exposure. that indicate risks to both humans and the environment, but to which degree is yet unknown.

Table 3. Compounds for which both human and ecotoxicological risk limits are derived and compared in this report. Ecotoxicological risk limits are reported in the EU-RAR for MTBE (EC, 2002) and Verbruggen et al.*, 2005 (all other compounds).*

CAS	Compound
71-36-3	1-butanol
123-86-4	*n*-butyl acetate
108-91-8	cyclohexylamine
111-46-6	diethylene glyol
141-78-6	ethyl acetate
107-21-1	ethylene glycol
67-56-1	methanol
78-93-3	methyl ethyl ketone
1634-04-4	methyl *tert*-butyl ether
75-25-2	tribromomethane
102-71-6	triethanolamine

2. Calculating Maximum Permissible Concentrations with Humanex

2.1 Background

The Humanex model calculates the exposure of humans to a substance, based on a combination of exposure routes from EUSES (EC, 1996) and CSOIL (Otte *et al*., 2001). The full procedure and details can be found in Bontje *et al.* (2005).

First, regional predicted environmental concentrations (PEC_{REG}) are calculated with EUSES. The substance properties and the relative emissions to different compartments (as determined by the industrial and use categories) determine how the substance partitions over the different environmental compartments.

The regional PECs calculated by EUSES are used as input in Humanex. The Humanex model only needs the relative importance of exposure routes. This is determined by the concentration ratios between the different environmental compartments (Van de Meent and De Bruijn, 1995). Therefore, the exact concentrations do not matter, but only the ratios between the different compartments and thus the PEC_{REG} can be based on a standard emission.

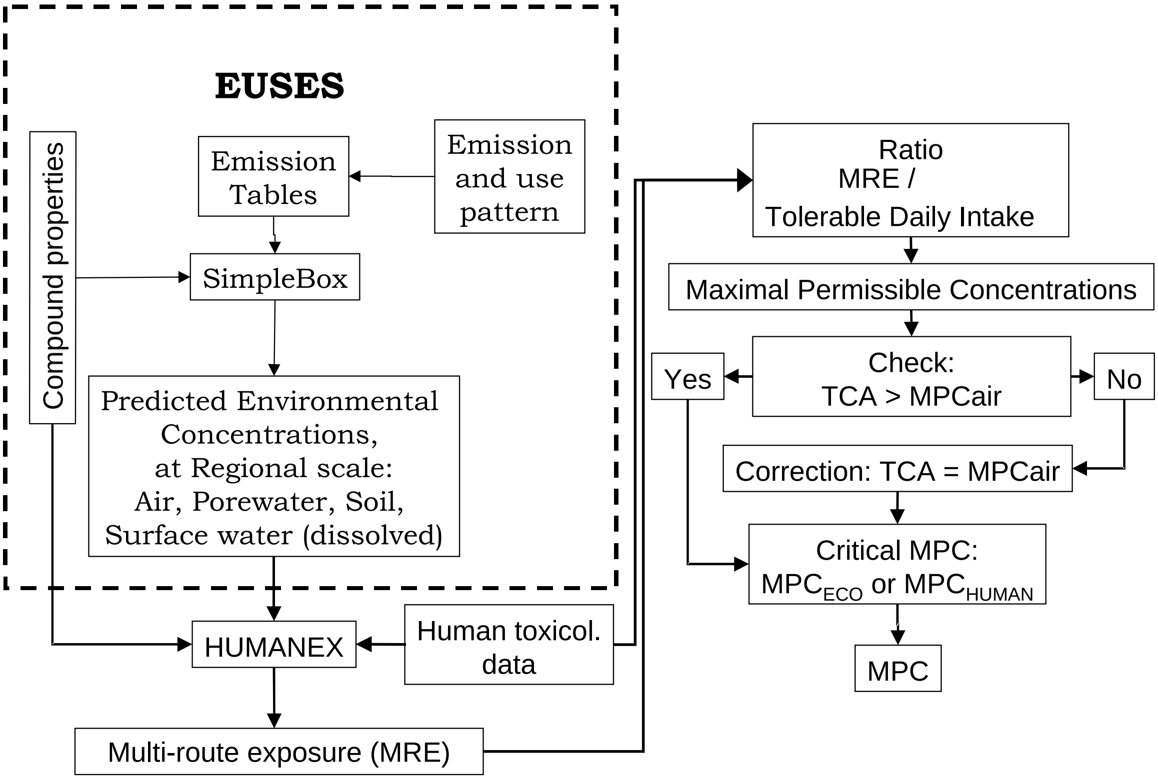


Figure 5. Diagram of the flow of information and decisions in the Humanex model. Humanex needs input from the EUSES model (indicated by the dashed box). TCA = Tolerable Concentration in Air; MPC = Maximum Permissible Concentration.

Second, the relative importance of exposure routes to humans is calculated from the PEC_{REG} as calculated by EUSES. The Multi-Route Exposure Estimate (MRE, [mg/day]) for humans is calculated from the standard emission (Figure 5, Table 4). The model then compares the MRE to the tolerable daily intake (TDI) of humans.

The third and final step in the calculation is based on the ratio of the TDI and the MRE. The concentrations (PEC_{REG}) must be proportionally adjusted until the MRE is equal to the TDI. When the MRE is equal to the TDI, the adjusted concentrations represent the MPC_{human} for each compartment. Thus, the final MPCs can be calculated based on the ratio of the TDI and the MRE:

$$MPC_{human,\ soil} = PEC_{REGsoil} * TDI/MRE$$
$$MPC_{human,\ air} = PEC_{REGair} * TDI/MRE$$
$$MPC_{human,\ surface\ water} = PEC_{REGsurface\ water} * TDI/MRE$$
$$MPC_{human,\ pore\ water} = PEC_{REGpore\ water} * TDI/MRE$$

MPC_{human} values are calculated for diethylene glycol (discussed later), to illustrate the mechanism for calculating MPCs as explained above (Table 4). The initial EUSES estimates are listed first, and are recalculated into the MPCs at the bottom of the table, based on the TDI/MRE ratio.

Table 4. Example MPC_{HUMAN} calculations for diethylene glycol. PEC_{REG} is initially based on a standard emission (100,000 t/a) and adjusted with the TDI/MRE ratio.

EUSES derived PEC_{REG}s for the compartments	**PEC_{REG} of the compartment**	**Conc.**	**Units**
Water – initial estimate	Surface water	9.46E+01	µg/L
Air – initial estimate	Air	5.10E-05	µg/m^3
Agricultural soil – initial est.	Soil	1.63E-01	µg/kg wwt
Sediment – initial estimate	Sediment	5.86E+01	µg/kg wwt
Agricultural pore water – initial estimate	Pore water	1.21E+00	µg/L
Calculated Total Exposure	MRE	2.73E+00	µg /kg bw/d
Tolerable Daily Intake	TDI	4.00E+02	µg /kg bw/d
Tolerable Conc. In Air	TCA	N.A.	µg/m^3
	TDI/MRE	1.46E+02	-/-
Maximum Permissible Concentrations for adult humans	$MPC_{human,\ surface\ water}$	1.39E+04	µg/L
	$MPC_{human,\ air}$	7.47E-03	µg/m^3
	$MPC_{human,\ soil}$ *	7.82E+01	µg/kg dwt
	$MPC_{human,\ sediment}$ *	2.63E+04	µg/kg dwt
	$MPC_{human,\ pore\ water}$	1.77E+02	µg/L

* Includes conversion from wwt to dwt according to Janssen *et al.* (2004).

2.2 Correction for the Tolerable Concentration in Air

In some cases, not only the TDI is available but also a Tolerable Concentration in Air (TCA). The TCA only concerns exposure by inhalation while the TDI is based on total dose received. These two values may be harmonized on the same dose basis, but this is not always known or possible. In such cases, a separate check on exceeding the TCA is performed. If the MPC_{air} > TCA, the previous calculated MPC_{air} is replaced by the value of the TCA (Table 5). In this example, the MPC for human risk was already calculated according to the procedure in section 2.1.

Table 5. Correction when MPC_{air} is higher than the TCA, illustrated for tetrahydrothiophene.

		Tetrahydrothiophene	**Units**
Maximum Permissible Concentrations for adult humans	$MPC_{surface\ water}$	9.95E+01	µg/L
	MPC_{air}	2.11E+03	µg/m^3
	MPC_{soil}	4.71E+00	µg/kg dwt
	$MPC_{pore\ water}$	4.87E+00	µg/L
TCA for tetrahydrothiophene		1.80E+2	µg/m^3
MPC_{air} higher than TCA?		yes	-/-
MCP_{air} = TCA	MPC_{air}	1.8E+2	µg/m^3

2.3 Integrating human and ecological risk limits

Humanex is based on multi-compartmental exposure. Humanex calculates maximum permissible concentrations (MPCs) in all compartments, corresponding to a human exposure that equals the maximum allowed dose or exposure. The maximum exposure is based on the acceptable daily intake (TDI) or tolerable concentrations in air (TCA) values as described below. If human exposure is less critical than exposure of ecosystems, the ecotoxicological MPC is also protective of humans. It is possible that some or all ecotoxicological MPCs are stricter than the corresponding human MPCs. For the example substance of tribromomethane (Table 6), the MPC_{eco} is lower than the MPC_{human} for the surface water compartment. For air, no MPC is available based on ecotoxicological data.

Table 6. Example calculation of critical MPCs for tribromomethane (CAS nr. 75-25-2).

	Surface water µg/L	Groundwater µg/L	Soil µg/kg dwt	Air µg/m^3
Eco	96	96	1061	-
Human	214	38	308	55
Ratio Eco/Human	0.45	2.5	3.4	-
Critical MPC	96	38	308	55

It is proposed to set the critical MPC as the final MPC for a compartment, to protect both ecosystems and humans from adverse effects of pollutants. This is similar to the reasoning in the framework of soil remediation (Van den Berg and Roels, 1995), where Serious Risk Concentrations (SRCs) are based on the most critical of human and ecotoxicological risk limits.

3. Integrating MPC_{human} with MPC_{eco}

3.1 Introduction

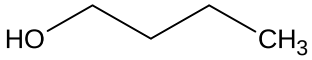
How humans are exposed to a substance is partly determined by the distribution of a substance over the different environmental compartments and food sources linked to those compartments (see Bontje *et al*., 2005). To calculate the relative contribution of exposure from the different environmental compartments, the physico-chemical parameters of a substance are needed as input for the model EUSES.
EUSES calculates the relative importance of exposure routes, as determined by the Predicted Environmental Concentrations for the compartments air, surface water, pore water and soil Another input for this calculation is information on the manufacture and use of a compound, to determine industry and use category.
This information was sourced from the internet and reviewed based on expert judgement (Van der Poel, pers. comm.). If no reliable information on type of use and emission characteristics is available, the EUSES worst-case option of 'wide dispersive use' is chosen.
All physicochemical parameters for the compounds are taken from the report on ecotoxicological risk limits for these substances (Verbruggen *et al*., 2005), and the EU-risk assessment report for MTBE (EC, 2002). Settings for EUSES are given in Appendix 2.
The human risk assessment compares the total intake from all exposure routes with previously derived TDI and TCA values. These were not derived in this report, but were taken from previously published sources. TDI and TCA values are summarized in Appendix 3.

MPC_{eco} values for surface water and soil (dry weight) are taken from the companion RIVM report (Verbruggen *et al*., 2005), except for MTBE (from EU-RAR: EC, 2002). Pore water is assumed to have the same MPC_{eco} as surface water. Further, calculated Maximum Permissible Concentrations based on the Humanex model (MPC_{human}) are for human adults and not adjusted for childhood years. The MPCs calculated in this chapter are based on all routes of exposure as presented in the introduction. The MPC_{human} values calculated with Humanex could be in conflict with MPC_{eco} or vice versa. The most critical MPC is identified and reported.

For each substance, a table is given that summarizes the main information for each substance. The TDI and the TCA (Appendix 3) are reported, as well as the MPC_{human} that is calculated with Humanex for the different compartments. The MPC_{eco} is shown and compared to the MPC_{human}, after which the most critical MPC is identified.
The contribution of the main compartments (surface water, ground water, air or soil) to human exposure is given as a percentage of total exposure. It should be realized that ingestion of e.g. leaf crops can be due to contaminant taken up by the plant either from air, from roots or both. The most important individual exposure route (cf. Figure 3) is shown at the bottom of the summary table. This percentage can be lower than the total percentage of the most dominant compartment, due to the summation of individual exposure routes.

3.2 Integration of risk limits

3.2.1 1-Butanol



Use, emission pattern and exposure

The largest uses of 1-butanol are industries that make butyl acrylate, meth-acrylate and other related chemicals. 1-Butanol is also added to solvents and detergent formulations. These use patterns are input to calculate environmental distribution of 1-butanol with EUSES (Appendix 2), using the substance properties from Appendix 1. 1-butanol is both highly volatile and soluble. The model results show, that the main routes of exposure to humans are surface water and air (Table 7). The main exposure routes of humans are drinking water (drw, 55.7%) and showering to a total of 58.1% and air (40.6%). Negligible contributions come from soil and root crops that take up the substance from pore water.

Table 7. MPC values for 1-butanol, and main routes of exposure to humans.

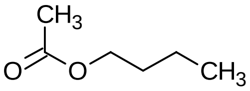
1-butanol	**TDI** (µg/kg bw/d)	**TCA** ($\mu g/m^3$)		**Corrected for TCA:**	
	1.25E+02	5.50E+02		NO	
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** ($\mu g/m^3$)	**Soil** (µg/kg dwt)	**Sediment** (µg/kg dwt)
MPCeco	2.24E+02	2.24E+02		1.49E+02	5.35E+02
MPChuman	2.43E+03	8.96E+02	1.71E+02	1.51E+03	7.74E+03
Ratio MPCeco/MPChuman	9.20E-02	2.50E-01		9.90E-02	6.92E-02
Critical MPC	2.24E+02	2.24E+02	1.71E+02	1.49E+02	5.35E+02
% importance of total exposure	58.047	1.281	40.668	0.003	
Dominant route of exposure	drw				
% of dominant route	55.647				

MPCs

The ecotoxicological MPC values for 1-butanol were derived previously. The Humanex calculations show that relatively high MPC_{human} values are estimated, as determined by total exposure from environment and food. For all compartments, the MPC_{eco} values are stricter, indicating that ecological risk is dominant over human risk for 1-butanol.

The MPC_{water} is determined by the MPC_{eco}, and therefore, the **MPC_{water}** does not need adjustment and is **224 µg/L.** The critical MPC groundwater is determined by the MPC_{eco} (set equal to the MPC for water, at **224 µg/L)**.
The MPC_{air} is determined by human exposure because no ecotoxicity data are available, and is calculated by Humanex based on the TDI and the distribution of 1-butanol over the environmental compartments. The **MPC_{air}** is set at **171 $\mu g/m^3$**. The critical **MPC_{soil} is 149 µg/kg dry wt** and is determined by ecological risk. This value is based on equilibrium partitioning (EqP) between water and soil. The critical $MPC_{sediment}$ is determined by EqP as well and is based on ecological risk (**535 µg/kg dry wt**).

3.2.2 *n*-Butyl acetate



Use, emission pattern and exposure

n-Butyl acetate is used as a precursor for polyethylene terephthalate (PET) plastic production and it is used as a solvent in the chemical and electronic industry. These use patterns are used to calculate environmental distribution of *n*-butyl acetate (Appendix 2), using the substance properties from Appendix 1.

Table 8. MPC values for n-butyl acetate, and main routes of exposure to humans.

_n_-butyl acetate	**TDI** (µg/kg bw/d)	**TCA** (µg/m^3)	**Corrected for TCA:**
	2.00E+02	1.00E+03	NO

	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µg/kg dwt)
MPC eco	1.80E+01	1.80E+01		9.57E+01	1.27E+02
MPC human	3.58E+02	1.09E+02	6.53E+02	5.93E+02	2.82E+03
Ratio MPC eco/MPC human	5.02E-02	1.65E-01		1.61E-01	4.49E-02
Critical MPC	1.80E+01	1.80E+01	6.53E+02	9.57E+01	1.27+02
% importance of total exposure	6.431	0.109	93.459	0.001	
Dominant route of exposure	air				
% of dominant route	93.265				

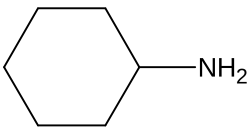
The MPC$_{eco}$ values for *n*-butyl acetate were derived in the companion report. The Humanex calculations (Table 8) show that the current risk limit for humans (TDI) correspond with MPC levels that are higher than those for ecosystems. Thus, MPCs for all compartments are determined by the ecotoxicological risk. The main exposure route of humans estimated by Humanex is air (93.5 %), drinking water and showering (6.4 %), due to the high vapour pressure and solubility of *n*-butyl acetate.

MPCs and integration

No additional calculations are necessary (all MPC$_{eco}$/MPC$_{human}$ *ratios* are < 1), and MPCs are determined by ecological risk in all cases except for air. This leads to the following integrated MPCs for *n*-butyl acetate:

The **MPC$_{water}$** is **18 µg/L,** the **MPC$_{groundwater}$** is **18 µg/L,** the **MPC$_{air}$** is **653 µg/m^3** the **MPC$_{soil}$** is **96 µg/ kg dry wt** and the **MPC$_{sediment}$** is **127 µg/ kg dry wt.**

3.2.3 Cyclohexylamine



Use, emission pattern and exposure

Cyclohexylamine is mostly used as a vulcanising agent, corrosion inhibitor and as an intermediate in the chemical industry for a diversity of chemicals. MPCs and exposure to humans is shown in Table 9. Most of human exposure (73.5%) originates from surface water through drinking water (including showering) and fish consumption. Exposure through air is not a main route of exposure, but substantial (25%). The MPC_{eco} is more stringent than MPC_{human} by four orders of magnitude. The missing compartments are integrated by the distribution pattern calculated by EUSES (Appendix 1).

Table 9. MPC values for cyclohexylamine, and main routes of exposure to humans.

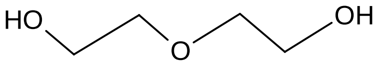
cyclohexylamine	**TDI** (µg/kg bw/d) 1.10E+04	**TCA** (µg/m^3) N.A.		**Corrected for TCA:** NO	
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µg/kg dwt)
MPC eco	2.00E-01	2.00E-01		8.12E-01	1.16E+00
MPC human	2.67E+05	9.46E+04	8.71E+03	1.47E+05	8.17E+05
Ratio MPC eco/MPC human	7.49E-07	2.11E-06		5.52E-06	1.42E-06
Critical MPC	2.00E-01	2.00E-01	8.71E+03	8.12E-01	1.16E+00
% importance of total exposure	73.495	1.616	24.886	0.003	
Dominant route of exposure	drw				
% of dominant route	69.516				

MPCs and harmonisation

For cyclohexylamine, all MPCs except air are determined by ecological risk.
The $\mathbf{MPC_{water}}$ is determined by the MPC_{eco} and is **0.2 µg/L.** The $MPC_{groundwater}$ is equal to the MPC_{eco} for water, **0.2 µg/L**. The $\mathbf{MPC_{human}}$ for air is **8710 µg/m^3**.
The $\mathbf{MPC_{soil}}$ (**0.81 µg/kg dry wt**) and the $\mathbf{MPC_{sediment}}$ (**1.2 µg/kg dry wt**) are determined by ecological risk, and are based on equilibrium partitioning (EqP) between water and soil or sediment.

Since all MPCs except for air are determined by the MPC_{eco}, and much lower than the corresponding MPC_{human}, it can be expected that a potential conflict exists between the $MPC_{eco, air}$ and the $MPC_{human, air}$. The $MPC_{eco, air}$ is not calculated from ecotoxicity studies, but similar to MPCs for sediment, it can be calculated based on partitioning coefficients. The $Kp_{,air-water}$ is calculated by EUSES from the ratio of concentrations in air to surface water (32.6 m^3/m^3). The $\mathbf{MPC_{eco, air}}$ is then **36 ng/m^3**, much lower than the $\mathbf{MPC_{human, air}}$ of **8710 µg/m^3**. In this case, the critical MPC_{air} is clearly determined by the ecotoxicological value.
In the EU, intercompartmental harmonisation is not considered. This viewpoint is now also integrated in the current national strategy for risk limit derivation. In this case, due to the very large difference (6 orders of magnitude) between MPC_{eco} and MPC_{human}, it can be expected that concentrations at the level of the $MPC_{human, air}$ could lead to exceeding MPC_{eco} values in water or soil due to intercompartmental exchange. However, if such concentrations will ever occur cannot be predicted in advance. The relevance of this process depends on local factors such as the magnitude, scale (local or regional) and duration of the hypothetical pollution event.

3.2.4 Diethylene glycol



Use, emission pattern and exposure

Diethylene glycol (DEG) is used for many applications such as anti-freezing agent, intermediate in the chemical industry, pH-regulating agent, fillers, solvents, etc. The TDI for DEG is a sum-TDI that includes DEG and ethylene glycol.

Exposure is mainly through the drinking water (drw) and very little exposure derived from the plant (Table 10). Plants take up DEG mainly from the air, but this is insignificant for total exposure. The MPC_{human} is almost a hundred times stricter than the MPC_{eco} in case of groundwater and soil.

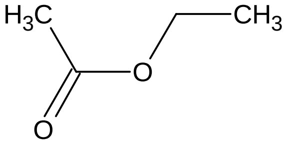
Table 10. MPC values for diethylene glycol and main routes of exposure to humans.

diethylene glycol	**TDI** (µg/kg bw/d)	**TCA** (µg/m^3)		**Corrected for TCA:**	
	4.00E+02	N.A.		NO	
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µg/kg dwt)
MPC eco	1.47E+04	1.47E+04		6.62E+03	3.20E+04
MPC human	1.39E+04	1.77E+02	7.47E-03	7.82E+01	2.63E+04
Ratio MPC eco/MPC human	1.06E00	8.32E+01		8.47E+01	1.22E+00
Critical MPC	1.39E+04	1.77E+02	7.47E-03	7.82E+01	2.63E+04
% importance of total exposure	99.796	0.166	0.038	0.000	
Dominant route of exposure	drw				
% of dominant route	98.977				

MPCs

In the case of diethylene glycol, all MPCs are determined by the risk for human health. The **MPC_{water}** is **14 mg/L**, the **$MPC_{groundwater}$** is **177 µg/L,** the **MPC_{air}** is **7.5 ng/m^3**, the **MPC_{soil}** is **78.2 µg/ kg dry wt**, and the **$MPC_{sediment}$** is **26.3 mg/ kg dry wt.**

3.2.5 Ethyl acetate



Use, emission pattern and exposure

Ethyl acetate is used as solvent for paints and as solvent in the chemical industry and a limited amount is produced as a foodstuff additive. Based on the Humanex calculations (Table 11), 89% of the total exposure originates from the air compartment through inhalation, while the remaining exposure is derived from surface water, by way of drinking water (9.7%) and showering (1.4%).

Table 11. MPC values for ethyl acetate and main routes of exposure to humans.

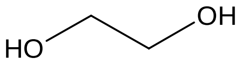
ethyl acetate	**TDI** (µg/kg bw/d)	**TCA** (µg/m^3)	**Corrected for TCA:**		
	9.00E+02	4.20E+03	NO		
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µg/kg dwt)
MPC eco	1.07E+02	1.07E+02		2.04E+02	3.89E+02
MPC human	3.04E+03	6.64E+02	2.79E+03	1.24E+03	1.03E+04
Ratio MPC eco/MPC human	3.53E-02	1.62E-01		1.64E-01	3.77E-02
Critical MPC	1.07E+02	1.07E+02	2.79E+03	2.04E+02	3.89E+02
% importance of total exposure	11.093	0.131	88.775	0.000	
Dominant route of exposure	air				
% of dominant route	88.563				

MPCs

No additional calculations are necessary because all MPC$_{eco}$/MPC$_{human}$ *ratios* are < 1. MPCs are determined by ecological risk in all cases except air. This leads to the following MPCs for ethyl acetate:

The **MPC$_{water}$** is **107 µg/L,** the **MPC$_{groundwater}$** is **107 µg/L,** the **MPC$_{air}$** is **2.8 mg/m^3** the **MPC$_{soil}$** is **204 µg/ kg dry wt** and the **MPC$_{sediment}$** is **389 mg/ kg dry wt.**

3.2.6 Ethylene glycol



Use, emission pattern and exposure

Ethylene glycol (EG) is used as an intermediate in the chemical industry, as anti freeze and as a solvent. Humanex calculations predict that human exposure is mainly by drinking water (drw; 97%) due to its high solubility and related high concentration in the surface water and relative low concentrations in the other compartments (Table 12).

Table 12. MPC values for ethylene glycol and main routes of exposure to humans. Drw=drinking water.

ethylene glycol	**TDI** (µg/kg bw/d)	**TCA** (µg/m^3)	**Corrected for TCA:**		
	4.00E+02	N.A.	NO		
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µ/kg dwt)
MPC eco	2.00E+05	2.00E+05		8.94E+04	4.34E+05
MPC human	1.36E+04	1.72E+03	2.25E+00	7.55E+02	2.57E+04
Ratio MPC eco/MPC human	1.47E+01	1.16E+02		1.18E+02	1.69E+01
Critical MPC	1.36E+04	1.72E+03	2.25E+00	7.55E+02	2.57E+04
% importance of total exposure	98.108	0.882	1.009	0.000	
Dominant route of exposure	drw				
% of dominant route	97.233				

MPCs

The TDI for EG is a sum-TDI that includes DEG and ethylene glycol. Similar to diethylene glycol, all MPCs for ethylene glycol are determined by the risk for human health. This leads to the following MPCs for ethylene glycol:

The **MPC$_{water}$** is **13.6 mg/L**, the **MPC$_{groundwater}$** is **1.72 mg/L**, the **MPC$_{air}$** is **2.25 µg/m^3**, the **MPC$_{soil}$** is **755 µg/ kg dry wt** and the **MPC$_{sediment}$** is **25.7 mg/kg dry wt**.

3.2.7 Methanol

$HO\text{-}CH_3$

Use, emission pattern and exposure

Methanol is used as a solvent for paints and chemical products in the industry and is mostly used as a precursor of formaldehyde. It is also used as an alternative non-fossil fuel. The relatively high partitioning to air explains the main exposure through air by inhalation of almost 47 % (Table 13). Exposure from leaf crops also originates indirectly from the air. Another important exposure pathway is by way of drinking water, because EUSES contains a relatively worst-case purification module.

Table 13. MPC values for methanol and main routes of exposure to humans.

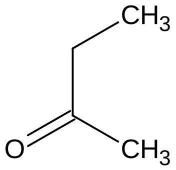
methanol	**TDI** (µg/kg bw/d)	**TCA** (µg/m^3)		**Corrected for TCA:**	
	5.00E+02	1.10E+03		NO	
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µg/kg dwt)
MPC eco	1.90E+02	1.90E+02		9.79E+01	4.26E+02
MPC human	8.06E+03	8.06E+03	8.16E+02	4.04E+03	1.58E+04
Ratio MPC eco/MPC human	2.36E-02	2.36E-02		2.42E-02	2.69E-02
Critical MPC	1.90E+02	1.90E+02	8.16E+02	9.79E+01	4.26E+02
% importance of total exposure	47.119	49.541	50.099	0.002	
Dominant route of exposure	air				
% of dominant route	46.645				

MPCs and integration

All MPC$_{eco}$/MPC$_{human}$ ratios are < 1, indicating that ecological risk dominates the calculations for the MPC. The only compartment determined by human risk is air. This leads to the following integrated MPCs for methanol:

The **MPC$_{water}$** is **190 µg/L**, the **MPC$_{groundwater}$** is **190 µg/L**, the **MPC$_{air}$** is **816 µg/m^3** the **MPC$_{soil}$** is **97.9 µg/ kg dry wt** and the **MPC$_{sediment}$** is **426 µg/ kg dry wt.**

3.2.8 Methyl ethyl ketone



Use, emission pattern and exposure

Methyl ethyl ketone (MEK) is largely used in professional paints and 'do-it-yourself'-paints, other applications are ink-solvents, intermediate in the chemical industry for e.g. organic synthesis and production of magnetic tapes. Often MEK is a by-product of acetic acid production. Again, high vapour pressure and high solubility combine into an exposure pattern through air (85%) and drinking water (from treated surface water; 12.8%, not shown in Table 14).

Table 14. MPC values for methy ethyl ketone and main routes of exposure to humans.

	TDI	**TCA**			
methyl ethyl ketone	(µg/kg bw/d)	(µg/m^3)		**Corrected for TCA:**	
	1.90E+02	8.75E+02		NO	
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µ/kg dwt)
MPC eco	1.20E+03	1.20E+03		2.21E+03	4.27E+03
MPC human	8.50E+02	4.12E+02	5.66E+02	7.32E+02	2.81E+03
Ratio MPC eco/MPC human	1.41E+00	2.91E+00		3.01E+00	1.52E+00
Critical MPC	8.50E+02	4.12E+02	5.66E+02	7.32E+02	2.81E+03
% importance of total exposure	13.918	0.379	85.702	0.001	
Dominant route of exposure	air				
% of dominant route	85.130				

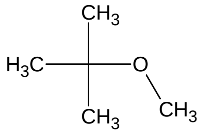
MPCs

MPC$_{eco}$/MPC$_{human}$ ratios all >1. This means that the risk for human health dominates for MEK. However, the values of the two types of risk limits are very similar.

This leads to the following MPCs for methyl-ethyl ketone:

The **MPC$_{water}$** is **850 µg/L**, the **MPC$_{groundwater}$** is **412 µg/L**, the **MPC$_{air}$** is **566 µg/m^3**, the **MPC$_{soil}$** is **732 µg / kg dry wt** and the **MPC$_{sediment}$** is **2.81 mg/ kg dry wt**.

3.2.9 Methyl *tert*-butyl ether



Use, emission pattern and exposure

Methyl *tert*-butyl ether (MTBE) is mainly used as a fuel additive. It serves as an anti-knocking agent and makes fuel burn more efficient. Negligible applications of MTBE are in the production of pharmaceuticals and production of isobutene. Exposure is mainly through air (79%), drinking water (17%) and some by showering (about 4%). Table 15 shows calculation details.

Table 15. MPC values for methy tert-*butyl ether and main routes of exposure to humans.*

methyl tert-butyl ether	**TDI** (µg/kg bw/d) 3.00E+02	**TCA** ($\mu g/m^3$) 2.60E+03	**Corrected for TCA:** NO		
	Surface water (µg/L)	**Groundwater** (µ/L)	**Air** ($\mu g/m^3$)	**Soil** (µg/kg dwt)	**Sediment** (µg/kg dwt)
MPC eco	2.60E+03	2.60E+03		2.40E+03	6.29E+03
MPC human	1.79E+03	5.60E+01	8.31E+02	7.36E+01	4.49E+03
Ratio MPC eco/MPC human	1.45E+00	4.64E+01		3.26E+01	1.40E+00
Critical MPC	1.79E+03	5.60E+01	8.31E+02	7.36E+01	4.49E+03
% importance of total exposure	20.798	0.034	79.168	0.000	
Dominant route of exposure	air				
% of dominant route	79.096				

Critical MPCs and integration

In the EU-RAR, the PNEC for MTBE is based on the lowest NOEC for *Mysidopsis bahia* with an assessment factor of 10. This PNEC of 2.6 mg/L is also the MPC_{water}. The MPC_{soil} is based on the MPC_{water} of 2.6 mg/L and is calculated at 0.77 mg/kg ww for the EU standard soil. The conversion to the Dutch standard and to dry weight yields an MPC_{soil} of 2.4 mg/kg dw. The $MPC_{sediment}$ is based on the EU-RAR value of 2.05 mg/kg ww. Here, the conversion for dry weight is a factor of 2.6 and the organic carbon conversion is 1.18, which results in an $MPC_{sediment}$ of 6.29 mg/kg dw.

The MPC_{human} is the limiting ERL for the integrated MPC to protect both humans and ecosystems. This leads to the following integrated MPC values:

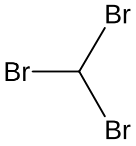
The **MPC_{water}** is **1.8 mg/L**, the **$MPC_{groundwater}$** is **56 µg/L**, the **MPC_{air}** is **831 $\mu g/m^3$** the **MPC_{soil}** is **73.6 µg/ kg dry wt** and the **$MPC_{sediment}$** is **4.5 mg/ kg dry wt**.

Comparison to Intervention values for MTBE

In the report by Swartjes *et al.* (2004), risk limits were derived for MTBE, based on the risk assessment concept for intervention values (Van den Berg and Roels, 1995). As detailed before, these limits are protective of situations where people are in contact with contaminated soil, either directly (ingestion) or indirectly (through food, inhalation etc.). The Humanex risk concept is based on the (worst-case) situation, where a substance is emitted in the environment and a steady-state concentration is reached for all compartments. It is also assumed that humans are exposed to this contaminated environment by all relevant routes, including food.

The reported risk limit for soil contamination is 221 mg/kg dry wt. This is a factor of 5 higher than the MPC$_{human, soil}$ at 73.6 µg/kg dry wt. This serves to illustrate that the concept of multi-media exposure, which leads to a summation of exposure routes to humans, is rather different from the CSOIL exposure concept.
For groundwater and surface water as a source for drinking water, the proposed risk limit for intervention values is 9420 µg/L. The MPC$_{human, water}$ is in the same order of magnitude, while the MPC$_{human, groundwater}$ calculated with Humanex is much lower at 56 µg/L.

3.2.10 Tribromomethane



Use, emission pattern and exposure

Tribromomethane, also known as bromoform, is used on a small scale mainly for in routine procedures to separate minerals, in laboratories, and in the electronics industry.
Tribromomethane is quite volatile and exposure is mainly through air (56.7%). Its high solubility explains the high concentration in groundwater / drinking water. Showering causes additional exposure (about 6%, not shown in Table 16).

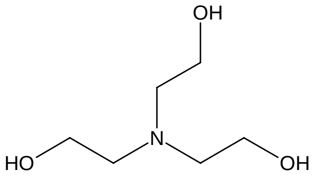
Table 16. MPC values for tribromomethane and main routes of exposure to humans.

tribromomethane	**TDI** (µg/kg bw/d)	**TCA** (µg/m^3)		**Corrected for TCA:**	
	2.00E+01	1.00E+02		NO	
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µg/kg dwt)
MPC eco	9.60E+01	9.60E+01		1.06E+03	1.23E+03
MPC human	2.14E+02	3.76E+01	3.97E+01	3.08E+02	2.26E+03
Ratio MPC eco/MPC human	4.49E-01	2.55E+00		3.44E+00	5.42E-01
Critical MPC	9.60E+01	3.76E+01	3.97E+01	3.08E+02	1.23E+03
% importance of total exposure	42.513	0.566	56.917	0.004	
Dominant route of exposure	air				
% of dominant route	56.710				

Critical MPCs and integration

Ecological risk dominates for tribromomethane for water and sediment. For groundwater and soil the risks for human health determine the MPC.
The **MPC$_{water}$** is equal to the MPC$_{eco}$ and is **96.0 µg/L.** The critical **MPC$_{groundwater}$** is determined by the MPC$_{human}$ and is **37.6 µg/L**. The critical **MPC$_{air}$** is determined by human exposure and is calculated at **39.7 µg/m^3**. The critical **MPC$_{soil}$** of **308 µg/kg dry wt** is determined by risk for human health. The critical **MPC$_{sediment}$** is determined by ecological risk, and is **1.23 mg/kg dry wt**, and is based on equilibrium partitioning (EqP) between water and soil.

3.2.11 Triethanolamine



Use, emission pattern and exposure

Triethanolamine contributes 15 to 20% of the total world production of ethanol amines. It is used as detergent, ingredient of cosmetics and fabric softener and is an intermediate in the production of ester quaternaries. Outside Europe triethanolamine is also used as antifreeze. Exposure to this compound is mainly from surface water, treated for drinking water (97%). Ecological risk dominates for this substance (Table 17).

Table 17. MPC values for triethanolamine and main routes of exposure to humans.

	TDI	**TCA**			
triethanolamine	(µg/kg bw/d)	(µg/m^3)		**Corrected for TCA:**	
	1.25E+04	5.00E+03		NO	
	Surface water (µg/L)	**Groundwater** (µg/L)	**Air** (µg/m^3)	**Soil** (µg/kg dwt)	**Sediment** (µ/kg dwt)
MPC eco	3.20E+02	3.20E+02		1.85E+02	7.37E+02
MPC human	4.25E+05	4.61E+04	1.24E-01	2.60E+04	8.60E+05
Ratio MPC eco/MPC human	7.52E-04	6.94E-03		7.12E-03	8.57E-04
Critical MPC	3.20E+02	3.20E+02	1.24E-01	1.85E+02	7.37E+02
% importance of total exposure	98.015	1.949	0.035	0.000	
Dominant route of exposure	drw				
% of dominant route	97.290				

Critical MPCs and integration

The **MPC$_{water}$** is determined by the MPC$_{eco}$ and is calculated at **320 µg/L**. The critical **MPC$_{groundwater}$** is also determined by the MPC$_{eco}$, set equal to the MPC for water, **320 µg/L.** The critical **MPC$_{air}$** is **0.12 µg/m^3** and determined by human exposure**.** No ecotoxicity data are available. The critical **MPC$_{soil}$** of **185 µg/kg dry wt** is determined by ecological risk, and is based on equilibrium partitioning (EqP) between water and soil.
The critical **MPC$_{sediment}$** is **737 µg/kg dry wt.**

4. Overview of risk limits

4.1 ERLs for water

Table 18. Overview of SRC and MPC values for water. All MPC_{human} values are calculated using the Humanex model.

Compound	SRC_{eco} (mg/L)	MPC_{eco} (µg/L)	MPC_{human} (µg/L)	Integrated MPC (µg/L)
1-butanol	**94**	224	2430	**224**
n-butylacetaat	**9.4**	18	358	**18**
Cyclohexylamine	**1.2**	0.20	2.67E+5	**0.20**
Diethylene glycol	**4083**	1.47E+4	1.39E+4	**13900**
Ethyl acetate	**66**	107	3040	**107**
Ethylene glycol	**2867**	2.00E+5	1.36E+4	**13600**
Methanol	**1218**	190	8060	**190**
Methyl ethyl ketone	**408**	1200	850	**850**
Methyl *tert*-butyl ether*	**47.5**	2600	1790	**1790**
Tribromomethane	**4.1**	96	214	**96**
Triethanolamine	**82**	320	4.25E+05	**320**

* = Based on the EU RAR (EC, 2002), SRC_{eco} from Swartjes *et al.* (2004).

For the compounds diethylene glycol, ethylene glycol, methyl ethyl ketone, and methyl *tert*-butyl ether the MPCs based on risks for human health are lower than those based on ecotoxicological risks, and determine the integrated MPC. For the other seven compounds, the ecotoxicological MPCs are lower.

4.2 MPCs for groundwater

Table 19. Overview of MPC values for ground water. All MPC_{human} values are calculated using the Humanex model.

Compound	MPC_{eco} (µg/L)	MPC_{human} (µg/L)	Integrated MPC (µg/L)
1-butanol	224	896	224
n-butyl acetate	18	109	18
cyclohexylamine	0.20	9.46E+4	0.20
diethylene glycol	1.47E+4	177	177
ethyl acetate	107	664	107
ethylene glycol	2.00E+5	1720	1720
methanol	190	8060	190
methyl ethyl ketone	1200	412	412
methyl *tert*-butyl ether*	2600	56	56
tribromomethane	96	38	38
triethanolamine	320	4.61E+04	320

* = Based on the EU RAR (EC, 2002).

For six substances, ecotoxicological risk is the dominant factor that determines the MPC. Human risk determines the MPC for diethylene glycol, ethylene glycol, methyl ethyl ketone, methyl *tert*-butyl ether, and tribromomethane.

4.3 MPCs for air

Table 20. Overview of MPC values for air. All MPC_{human} values for air are calculated using the Humanex model.

Compound	MPC_{eco} (µg/L)	MPC_{human} (µg/L)
1-butanol	-	171
n-butyl acetate	-	653
cyclohexylamine	-	8710
diethylene glycol	-	7470
ethyl acetate	-	2790
ethylene glycol	-	2.25
methanol	-	816
methyl ethyl ketone	-	566
methyl *tert*-butyl ether	-	831
tribromomethane	-	39.7
triethanolamine	-	0.12

No separate MPC_{eco} were derived and compared to MPC_{human} values. In principle, this could be done using EUSES. The same principles that are used to calculate the relative importance of exposure routes for humans could be used to calculate the $MPC_{eco,\ air}$. This is shown in the calculations for cyclohexylamine (section 3.2.3). Because $MPC_{eco,\ air}$ values are not formally required, no comparison was made. Section 3.2.3 shows that this could, in exceptional cases, lead to problems due to intercompartmental transfer.

4.4 MPCs for soil

Table 21. Overview of SRC and MPC values for soil. All MPC_{human} values are calculated using the Humanex model.

Compound	SRC_{soil} (mg/kg)	$MPC_{eco,\ soil}$ (µg/kg dw)	$MPC_{human,\ soil}$ (µg/kg dw)	Integrated MPC (µg/kg dw)
1-butanol	63	149	1510	149
n-butyl acetate	50	96	593	96
cyclohexylamine	5.0	0.81	1.47E+5	0.81
diethylene glycol	1838	6624	78.2	78.2
ethyl acetate	125	204	1240	204
ethylene glycol	1282	8.94E+4	755	755
methanol	627	98	4040	98
methyl ethyl ketone	749	2205	732	732
methyl *tert*-butyl ether	44	2400	74	74
tribromomethane	46	1061	308	308
triethanolamine	47	185	2.6E+4	185

Similar to groundwater, human risk determines the MPC_{soil} for diethylene glycol, ethylene glycol, methyl ethyl ketone, methyl *tert*-butyl ether, and tribromomethane. For the other six substances, ecotoxicological risk is the dominant factor that determines the MPC.

4.5 MPCs for sediment

Table 22. Overview of SRC and MPC values for sediment. All MPC_{human} values are calculated using the Humanex model.

Compound	$SRC_{eco, sed}$ (mg/kg)	$MPC_{eco, sed}$ (µg/kg)	$MPC_{human, sed}$ (µg/kg)	Integrated MPC (µg/kg dw)
1-butanol	226	535	7740	535
n-butyl acetate	66	127	2820	127
cyclohexylamine	7.2	1.2	8.17E+5	1.2
diethylene glycol	8883	3.20E+4	2.63E+4	2.63E+4
ethyl acetate	239	389	1.03E+4	389
ethylene glycol	6230	4.34E+5	2.57E+4	2.57E+4
methanol	6729	426	1.58E+4	426
methyl ethyl ketone	1452	4275	2810	2810
methyl *tert*-butyl ether	116 *	6300*	4490	4490
tribromomethane	53	1225	2260	1225
triethanolamine	188	737	8.60E+5	737

* In Swartjes *et al.* (2004), ERLs were determined with the same value for soil and sediment. However, soil and sediment have different characteristics (organic carbon content, water content, density). These are taken into account in the current tables.

Similar to surface water, the MPC_{human} is lower than the MPC_{eco}. for diethylene glycol, ethylene glycol, methyl ethyl ketone, and methyl *tert*-butyl ether. For the other seven substances, ecotoxicological risk is the dominant factor that determines the MPC.

5. Discussion

5.1 MPCs protective for man and ecosystems

This report is an attempt to compare human and environmental risk limits and derive integrated MPCs. This study shows that, for a heterogeneous set of substances, environmental risk limits are often protective of humans as well. In several cases however, human risk leads to more stringent risk limits (Tables 18-22). In most cases, integrating the two types of MPCs does not lead to much lower MPC values. In some cases, the MPC_{human} values are more than an order of magnitude lower, e.g. diethylene glycol MPCs for groundwater (Table 19). In these cases, it should be checked if that compartment is an important exposure source for humans. If so, downward adjustment of the MPC may be warranted. Some subtleties exist when calculating a coherent set of MPCs for human exposure that will be discussed below.

5.2 The interpretation of MPC_{human} values

MPC_{human} values derived in the INS project protect humans against exposure to all environmental compartments *simultaneously*. This includes transfer of substances from the environment to food and drinking water. The actual exposure from each compartment of course depends on substance properties but also on how substances are produced, used and emitted (see Bontje *et al*., 2005). MPCs should protect man and ecosystems against adverse effects. The goal of the current study is, to calculate *background* levels, if a substance is emitted from diffuse sources and on a regional scale. These risk limits therefore have a different interpretation than those derived in the framework of intervention values (Van den Berg and Roels, 1995). In the latter case, the limits should protect man from adverse effects of living on a contaminated soil.

The correct interpretation of MPC_{human} values is, that these concentrations protect man against diffuse emissions of a substance (on a regional scale), *assuming* that the substance has partitioned over all environmental phases. Each environmental phase contributes to the overall exposure of man.
In the case of volatile substances that are also highly soluble, as for some substances in this report, air and drinking water exposure are the dominant routes of exposure. In the Humanex calculations, concentrations in all compartments are in steady-state, based on the properties of the chemical and the environmental phases. This can result in seemingly puzzling results. The MPC_{human} for soil for such substances is low when compared to the SRC_{human}, as can be seen for MTBE (section 3.2.9). This is not because soil is the most important exposure route, but only because a steady-state is assumed between these phases and the partitioning coefficient from air to soil is low due to the substance properties.

This example shows that MPC_{human} values should be interpreted with care. MPC_{human} values should be regarded as a set of coherent concentrations for all compartments that protect man against diffuse, regional emissions of substances. The current framework for local soil contamination that is used in the Netherlands leads to risk limits that have a different value and different interpretation than MPC values. In local contamination situations, non-equilibrium conditions exist that require a different approach than the one in this report, taking local conditions and background concentrations into account. The soil contamination framework and the current framework have different goals and should be considered as tools that complement each other.

5.3 Exposure assumptions and uncertainty

Large quantitative differences exist between the predictions of various human exposure models (Swartjes *et al*., 2002). The current approach is certainly not the only valid one. It should be realized that some assumptions that are taken in the EUSES model are typically worst-case, such as the relatively low efficiency of drinking water purification, the assumption that all food is produced in the region where emissions occur etc. (see Bontje *et al*., 2005) for an overview and discussion of these model assumptions). However, when not much is known about actual cumulative exposure of humans to a substance, a worst-case approach is fitting for a general risk limit such as the MPC that should protect against chronic, 24h, life-time exposure to a substance. In a more detailed, site-specific (local) analysis, some or several of the assumptions on exposure routes could be falsified (e.g., no exposure to contaminated drinking water), allowing a higher exposure by the remaining exposure routes. This means that exceeding the MPC_{human} in a certain compartment will only present a risk if the concentrations of that substance in other compartments are equal or higher to the MPC_{human} as calculated in this report. If this is not the case, (some) compensation may occur if other exposure routes are less important than is assumed in the steady-state calculations. Policy action when risk limits are exceeded in the framework of the method presented here, thus requires access to the full set of MPCs (both MPC_{eco} and MPC_{human}) to determine if exposure is within the limits of the set of MPCs.

A more detailed analysis may be needed to determine the dominant sources of exposure to humans in a local pollution situation. In that case, the exposure profile and MPCs calculated by Humanex can be compared to local concentrations to identify the most likely exposure routes.

The concentrations that are calculated by EUSES are harmonized over the different compartments. For the calculation of the exposure of humans, who are exposed via several routes simultaneously, this is necessary. It can be argued that comparing both human-toxicological and ecotoxicological MPC values and taking the lowest value as the final value, in analogy with the risk assessment according to the Technical Guidance Document (TGD), is more conservative than strictly necessary. It is however the easiest way to compare risk limits without the need for further details. Alternatively, one could only use the MPC_{human} for the compartments emerging from the dominant exposure routes as indicated by Humanex, neglecting the contribution of other compartments. In that case, MPCs would only be determined by human risk if the MPC_{human} is lower than the MPC_{eco}, and represent a major part (percentage to be determined) of total exposure.

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The results as presented in this report have been discussed by the members of the scientific advisory group (WK-INS), who are acknowledged for their contribution and comments. The advisory group provides a non-binding scientific comment on the final draft of a report in order to advise the Steering Committee for Substances on the scientific merits of the report.

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Appendix 1 Substance properties used

Compound	Group	Cas	MW	log K_{ow}	log K_{oc}	SOL (mg/L)	T. Melt °C.	T. Boil °C.	Vp (Pa) 20 to 25 °C	Henry (Pa.m^3.mol^{-1})
1-butanol	E	71-36-3	74.12	0.88	1.35	73633	-62.33	117	914	0.85
n-butyl acetate	D	123-86-4	116.16	1.78	1.94	9559	-56.83	125	1673	28.51
cyclohexylamine	E	108-91-8	99.18	1.307	1.307	1000000	-27.11	134	1346	0.421
diethylene glycol	B	111-46-6	106.12	-1.31	-0.011	1000000	9	245	0.89	0.000203
ethyl acetate	E	141-78-6	88.11	0.73	1.408	79710	-82.08	77	8807	15.2
ethylene glycol	B	107-21-1	62.07	-0.54	-0.0304	1000000	-31.62	197	11.22	0.00608
methanol	C	67-56-1	32.04	-0.77	0.297	1000000	-101	650	16652	0.452
methyl ethyl ketone	E	78-93-3	72.11	0.29	1.381	218562	-80.48	80	12316	5.13
methyl tert-butyl ether	E	1634-04-4	88.15	1.06	1.05	42000	-94.3	55	33458	43.8
tetrahydriothiophene	D	110-01-1	88.17	1.79	1.953	3730	-48.82	84	3890	61.9
tribromomethane	D	75-25-2	252.73	2.67	2.13	3115	-11.87	158	727	57.97
triethanolamine	A	102-71-6	149.19	-1	0.489	1000000	21.6	335	0.00856	3.42E-14

Substance properties as tabulated above, are taken from RIVM report 601501016 (Verbruggen *et al*., 2005), except for MTBE (EC, 2002).

Appendix 2 EUSES settings for calculations of PECREGs

EUSES version 1.00 was used with settings as follows:

- Production volumes for all compounds are assumed to be 10^5 ton/year, unless stated otherwise.
- Regional production volume of substance was assumed to be 10% of total production volume of the chemical in the EU, unless stated otherwise.
- The settings for the default country (regional scale) were changed to resemble the Netherlands:

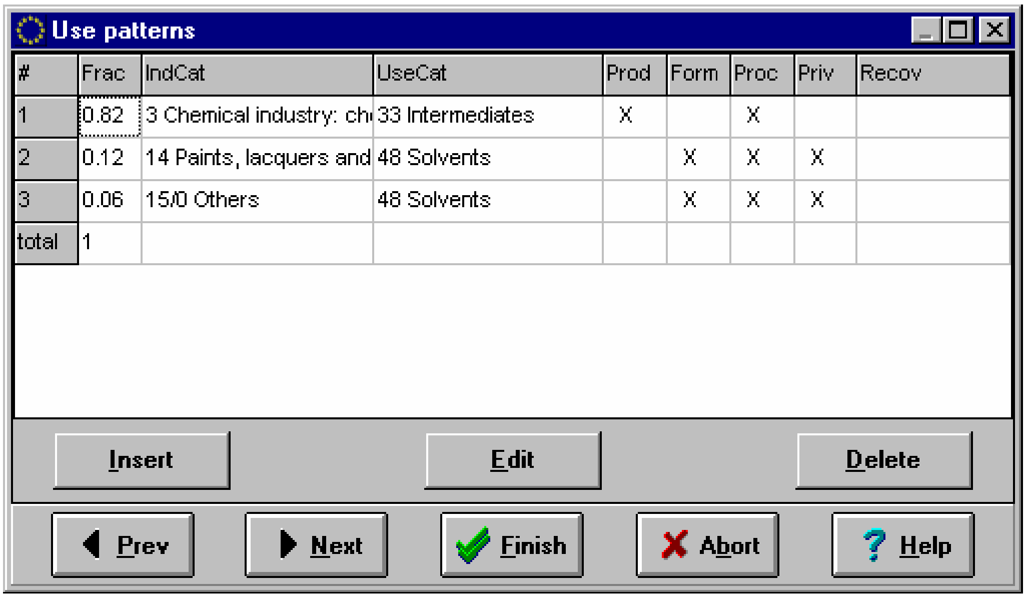
	Point estimate	Range
natural soils	0.152658004	10-25
agricultural soil	0.626077326	40-75
industrial soil	0.118765798	5-20
Water1	0.102499508	8-12

- The input into the Humanex model are the following concentrations:
  - PEC_{REG} surface water (dissolved) mg/L
  - PEC_{REG} air (total) mg/m^3
  - PEC_{REG} agricultural soil (total) mg/kg_{wwt}
  - PEC_{REG} sediment (total) mg/kg_{wwt}
  - PEC_{REG} in pore water of agricultural soils mg/L

1-Butanol

High Production Volume: Yes

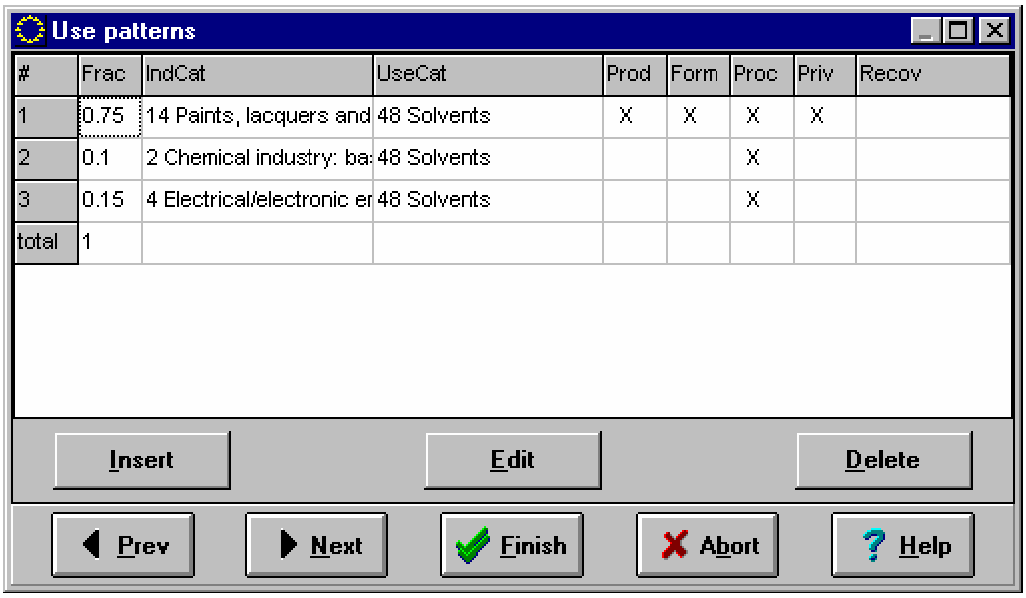
Regional production volume of substance: 10% of Production volume of chemical in EU



#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.82	3 Chemical industry: ch	33 Intermediates	X		X		
2	0.12	14 Paints, lacquers and	48 Solvents		X	X	X	
3	0.06	15/0 Others	48 Solvents		X	X	X	
total	1							

n-Butyl acetate

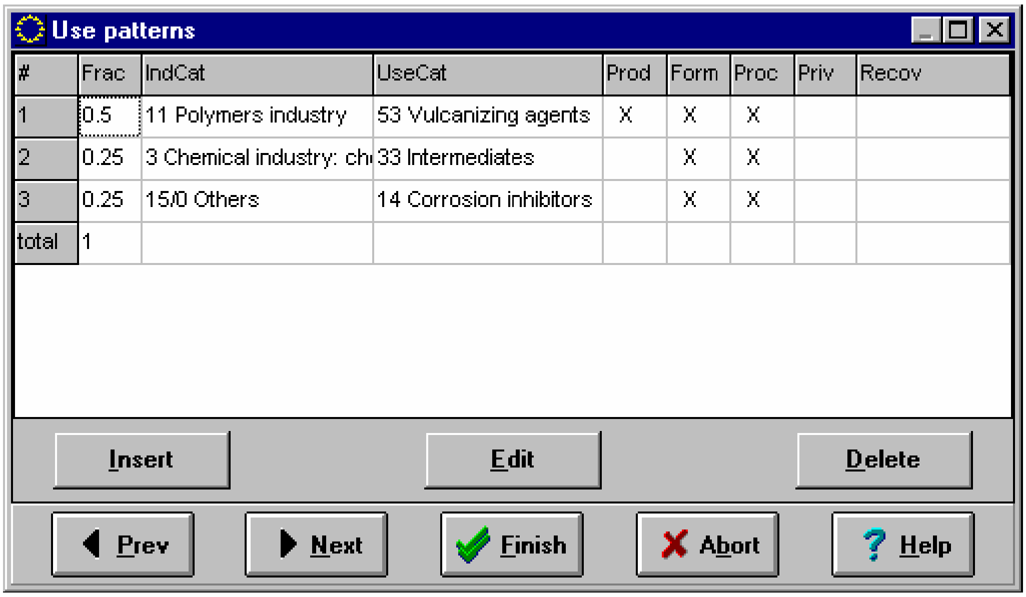
High Production Volume: Yes
Regional production volume of substance: 10% of Production volume of chemical in EU



#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.75	14 Paints, lacquers and	48 Solvents	X	X	X	X	
2	0.1	2 Chemical industry: ba:	48 Solvents			X		
3	0.15	4 Electrical/electronic er	48 Solvents			X		
total	1							

Cyclohexylamine

High Production Volume: Yes
Regional production volume of substance: 10% of Production volume of chemical in EU

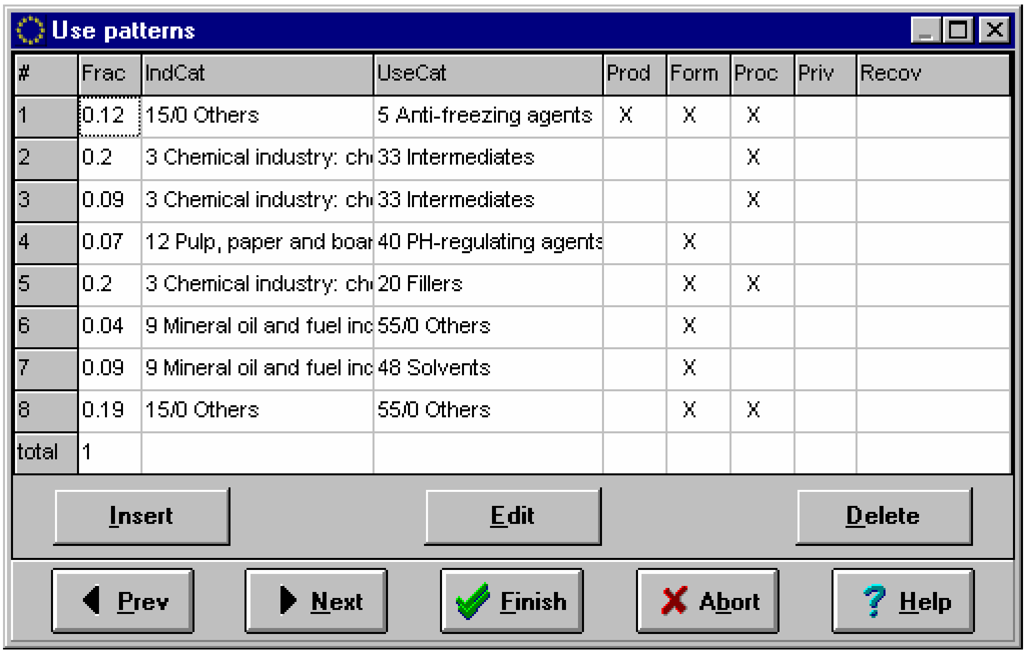


#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.5	11 Polymers industry	53 Vulcanizing agents	X	X	X		
2	0.25	3 Chemical industry: ch	33 Intermediates		X	X		
3	0.25	15/0 Others	14 Corrosion inhibitors		X	X		
total	1							

Diethylene glycol

High Production Volume: Yes

Regional production volume of substance: 10% of Production volume of chemical in EU

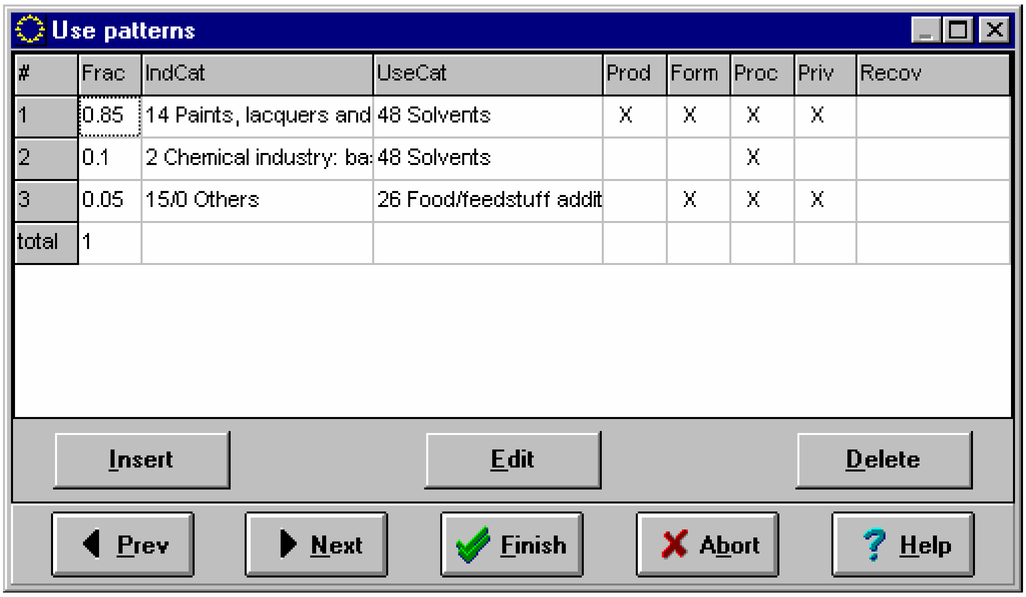


#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.12	15/0 Others	5 Anti-freezing agents	X	X	X		
2	0.2	3 Chemical industry: chi	33 Intermediates			X		
3	0.09	3 Chemical industry: chi	33 Intermediates			X		
4	0.07	12 Pulp, paper and boar	40 PH-regulating agents		X			
5	0.2	3 Chemical industry: chi	20 Fillers		X	X		
6	0.04	9 Mineral oil and fuel inc	55/0 Others		X			
7	0.09	9 Mineral oil and fuel inc	48 Solvents		X			
8	0.19	15/0 Others	55/0 Others		X	X		
total	1							

Ethyl acetate

High Production Volume: Yes

Regional production volume of substance: 10% of Production volume of chemical in EU

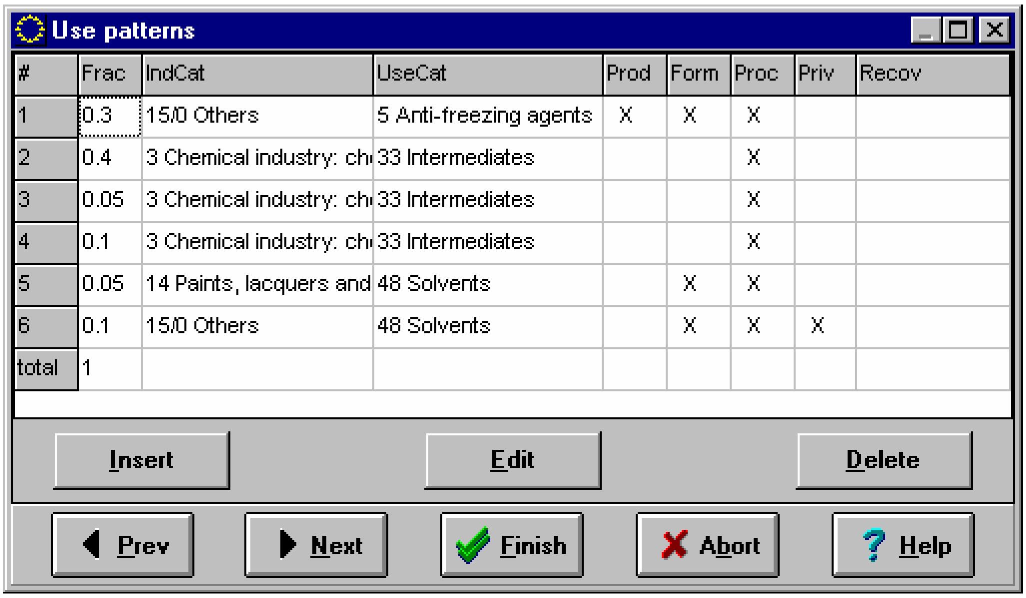


#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.85	14 Paints, lacquers and	48 Solvents	X	X	X	X	
2	0.1	2 Chemical industry: ba	48 Solvents			X		
3	0.05	15/0 Others	26 Food/feedstuff addit		X	X	X	
total	1							

Ethylene glycol

High Production Volume: Yes

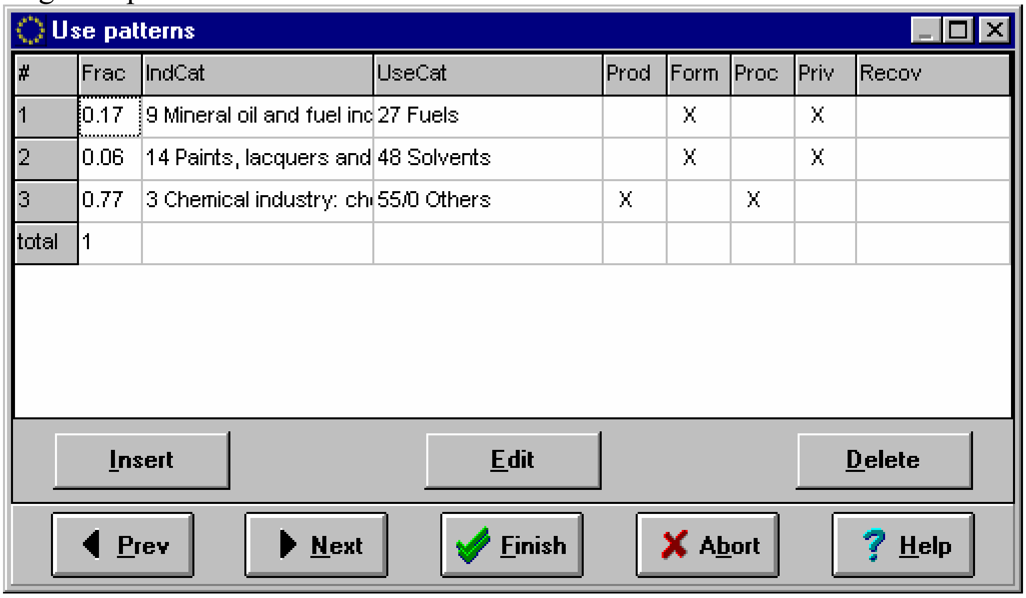
Regional production volume of substance: 10% of Production volume of chemical in EU



#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.3	15/0 Others	5 Anti-freezing agents	X	X	X		
2	0.4	3 Chemical industry: ch	33 Intermediates			X		
3	0.05	3 Chemical industry: ch	33 Intermediates			X		
4	0.1	3 Chemical industry: ch	33 Intermediates			X		
5	0.05	14 Paints, lacquers and	48 Solvents		X	X		
6	0.1	15/0 Others	48 Solvents		X	X	X	
total	1							

Methanol

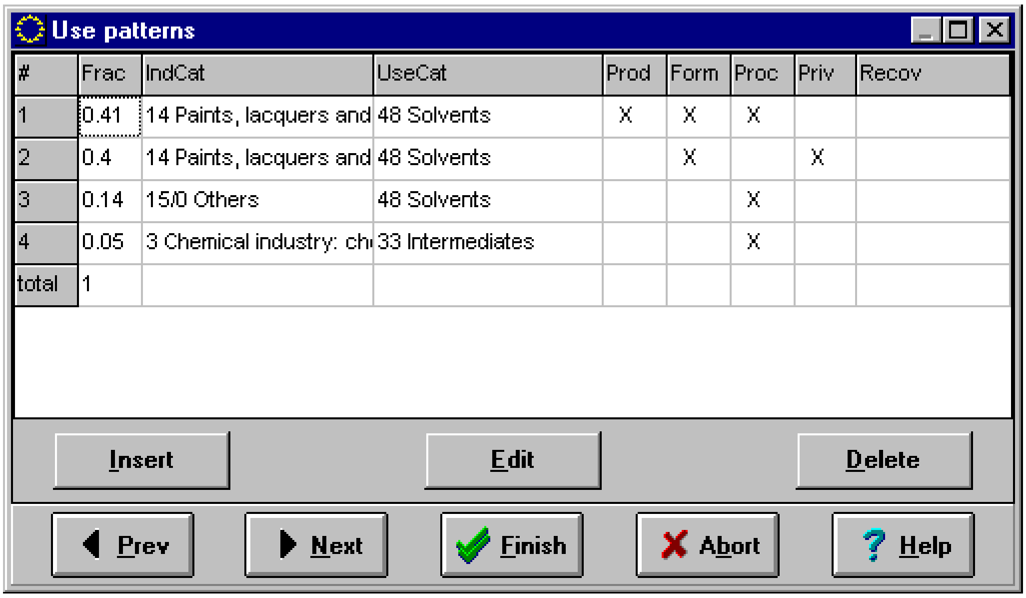
High Production Volume: Yes
Regional production volume of substance: 10% of Production volume of chemical in EU



#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.17	9 Mineral oil and fuel inc	27 Fuels		X		X	
2	0.06	14 Paints, lacquers and	48 Solvents		X		X	
3	0.77	3 Chemical industry: ch	55/0 Others	X		X		
total	1							

Methyl ethyl ketone (MEK)

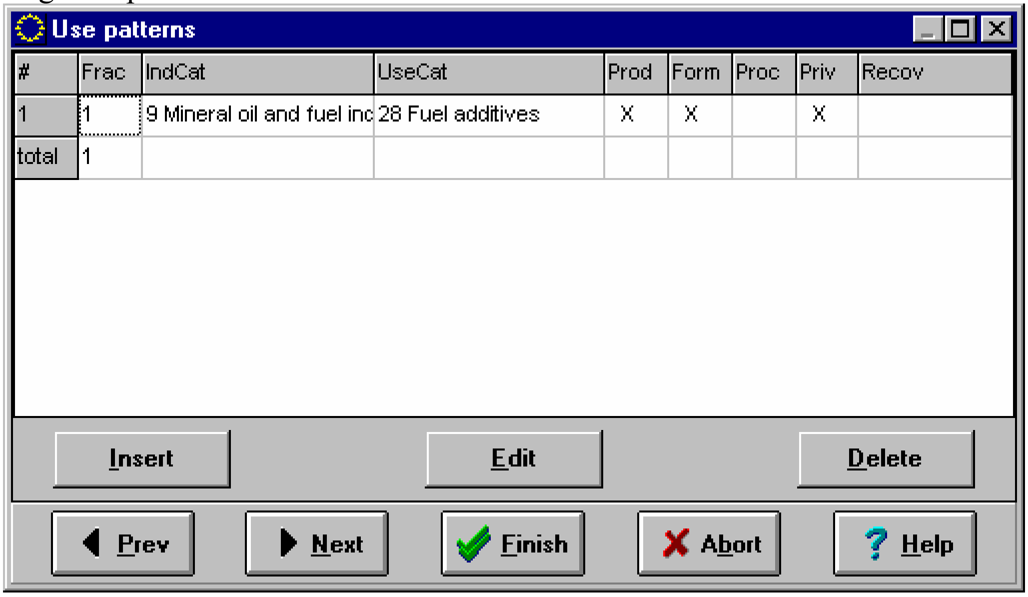
High Production Volume: Yes
Production volume of chemical in EU: 1×10^6 ton/year NOT 1×10^5 ton/year
Regional production volume of substance: 2.22×10^5 ton/year NOT 10% of Production volume of chemical in EU



#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.41	14 Paints, lacquers and	48 Solvents	X	X	X		
2	0.4	14 Paints, lacquers and	48 Solvents		X		X	
3	0.14	15/0 Others	48 Solvents			X		
4	0.05	3 Chemical industry: ch	33 Intermediates			X		
total	1							

Methyl *tert*-butyl ether (MTBE)

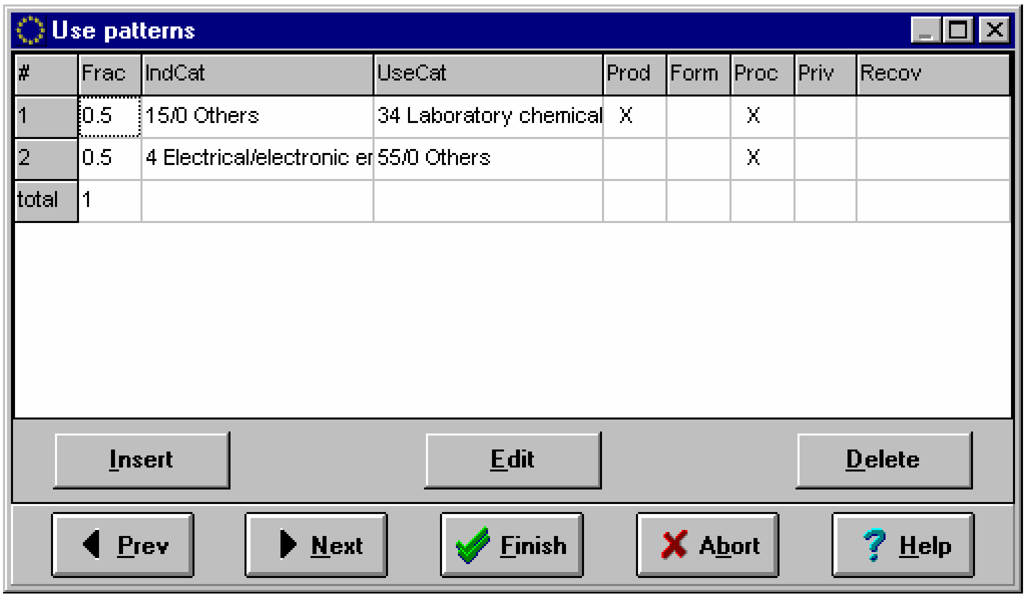
High Production Volume: Yes
Regional production volume of substance: 10% of Production volume of chemical in EU



#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	1	9 Mineral oil and fuel inc	28 Fuel additives	X	X		X	
total	1							

Tribromomethane (bromoform)

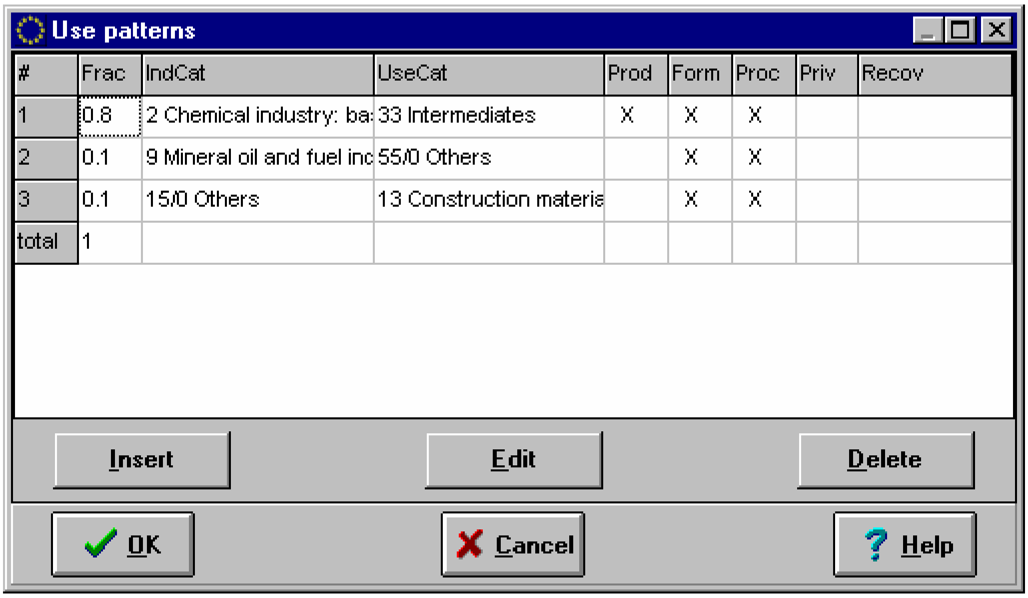
High Production Volume: Yes
Regional production volume of substance: 10% of Production volume of chemical in EU



#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.5	15/0 Others	34 Laboratory chemical	X		X		
2	0.5	4 Electrical/electronic er	55/0 Others			X		
total	1							

Triethanolamine

High Production Volume: Yes
Regional production volume of substance: 10% of Production volume of chemical in EU



#	Frac	IndCat	UseCat	Prod	Form	Proc	Priv	Recov
1	0.8	2 Chemical industry: ba	33 Intermediates	X	X	X		
2	0.1	9 Mineral oil and fuel inc	55/0 Others		X	X		
3	0.1	15/0 Others	13 Construction materia		X	X		
total	1							

Appendix 3 Tolerable Daily Intakes and Tolerable Concentrations in Air

CAS	Compound	MTR		Reference	Remark
		TDI[a]	TCA[b]		
75-25-2	Bromoform	20	100 (p)[c]	Janssen *et al.* (1998)	
71-36-3	1-Butanol	125	550 (p)	Janssen *et al.* (1995)	
123-86-4	*n*-Butyl acetate	200 (p)	1000	Janssen *et al.* (1995)	
108-91-8	Cyclohexylamine	11000	NA[d]	EU (1996)	miscible; basic
111-46-6	Diethylene glyol	400[e]	NA	Janssen *et al.* (1995)	miscible
141-78-6	Ethyl acetate	900	4200 (p)	Janssen *et al.* (1998)	
107-21-1	Ethylene glycol	400[e]	NA	Janssen *et al.* (1995)	miscible
67-56-1	Methanol	500	1100	Janssen *et al.* (1995)	miscible
1634-04-4	Methyl *tert*-butyl ether	300	2600	MTBE-RAR (ECB, 2002)	
78-93-3	Methyl ethyl ketone	190 (p)	875	Janssen *et al.* (1995)	
102-71-6	Triethanolamine	12500[f]	5000[f]		miscible; basic

MTR= Maximum Tolerable Risk level

[a] TDI (Tolerable Daily Intake) in $\mu g/kg_{bw}/d$

[b] TCA (Tolerable Concentration in Air) in $\mu g/m^3$

[c] p = provisional values

[d] NA = Not available

[e] Sum-TDI applicable for ethylene glycol and diethylene glycol

[f] Provisional data, from OECD SIDS (triethanolamine)

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