



Working procedure for conducting site and application specific Environmental Risk Assessment of chemicals:

Mining & Asphalt application

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ABSTRACT

This report was made within the project DANTEs that is supported by the EU Life Environment Programme.

Objective

The objective of this report is to present a working procedure for conducting Environmental Risk Assessments for specific applications based on two case studies. The working procedure is not intended for the regulatory type of Risk Assessment as laid out in the Directive 93/67/EEC and Regulation 1488/94.

The first ERA is an application and site specific analysis of the risks a chemical used in mining applications poses to the groundwater and river water.

The second ERA assesses risks to the local environment surrounding roads, posed by the construction and use phases of an asphalt application.

Result

The risk assessment case studies described in this report are two approaches to find the limitations and hotspots for further work. The working procedure developed based on these case studies can be used as a starting point and a framework for other ERAs of this kind (i.e. looking at specific applications of a chemical).

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1 GENERAL INTRODUCTION

This report was made within the project DANTES that is supported by the EU Life Environment Programme.

This report presents two case studies, a mining and an asphalt application, and a working procedure for conducting initial Environmental Risk Assessments (ERAs) based on these specific applications. The working procedure is not intended for Risk Assessments according to the EU regulatory framework although the recommendations in the Technical Guidance Document (TGD) are often applied in the case studies. The references to the TGD refer to Part II, chapter 3 "Environmental Risk Assessment".

The intended users of this report are anyone interested in ERA in the EU, through the DANTES project. More information about ERA can be found under "Assessment tools" on www.dantes.info or in the report "Methods and Tools for Assessment of Environmental Risk" (found under Publications on www.dantes.info).

These initial or screening risk assessments are based on available data, site specific parameters and use many worst-case assumptions. The reason for making these kind of site specific Risk Assessments can be that an initial Risk Assessment for all applications of a chemical has shown that there may be problems with a specific application and it therefore has to be looked into further. Another reason may be that authorities require a Risk Assessment to be made e.g. as part of an Environmental Impact Assessment for a production site.

When risk quotients (RCR), which result from the comparison of exposure and effects, are higher than 1 these worst-case assumptions should be refined. It should always be kept in mind that the quality and number of data always determine the usefulness of an ERA.

2 WORKING PROCEDURE

This working procedure is based on experiences from the two case studies presented in chapter 3 and 4.

The following procedure can be used to try to find the concentrations of chemical to which the environment may be exposed.

2.1 Finding the routes of release

1. Try to find information on how the chemical or product containing the chemical is used and handled and in which quantities. Also try to find information on the geography and lay-out of the site, process or application.
Make a picture or map of the site, process or application and find the flows of the chemical in this picture.
2. By looking at this picture or map and considering how the chemical is handled; how and where can the chemical reach the environment and in which quantities or concentrations?
 - By air or water?
 - To water treatment plant?
 - Continuous, intermittent or single release?

Result: a schematic picture or map that includes all of the flows of the chemical with quantities and all of the possible releases to the surrounding environment.

2.2 Modelling the exposure

3. Once the chemical is in the environment, how does it spread?
Based on how and where the chemical can reach the environment, information on the site specific environmental conditions at these release points is needed. The information can include temperatures, soil type(s) and their hydrological conductivity, water flows and temperatures, distances between the points of release and species or other things of interest to protect, e.g. a river, a water protection area or the ground water.
Try also to find all information about the physico-chemical properties of the chemical, especially the K_{OW} , volatility, molecular weight and degradability (biodegradation, photolysis and hydrolysis).
Result: a list of all of the available environmental information about the points of release and the physico-chemical properties.
4. Work out a model of how the chemical spreads and how it is distributed between air, water, soil and sediment (whichever is relevant at the different release points) based on information about the environmental conditions. The TGD can give guidance on how to model chemicals in the environment. EUSES [7] is a software tool that also can be used to model the exposure of a chemical, but it needs to be set with the site specific conditions, otherwise it will use default EU parameters.
Use site specific information on the needed parameters, e.g. hydrological conductivity or depth to ground water. If no site specific information is available,

try to find more general information about the area such as type of soil normally found in the area, or as a last resort use average data for the EU (which is included in the EUSES model).

Use chemical specific data on physico-chemical properties. If no chemical specific data is available, the TGD has guidance on how to calculate certain parameters from the structure of the molecule using so called (Q)SAR (Quantity Structure Activity Relationships). A simple QSAR computer program that has been developed by the US EPA, called EPISuite, can be found on the internet and downloaded for free.[3]

There are some software models that can be used for modelling a chemical release in a river, such as CORMIX or Visual Plumes.

Air releases can be dealt with by using the EUSES model, but generally the air releases are spread out over such a large area that the concentrations become very low and do therefore not constitute a risk to the environment. If the chemical is toxic and very persistent it can accumulate in the environment and reach toxic concentrations in the environment as well as in species higher up in the food chain.

Result: Predicted Environmental Concentrations (PECs) for the compartments water, sediment and soil, at the different release points.

2.3 Determining the effect levels

5. Try to find as much information on the eco-toxicity of the chemical as possible. Safety factors, called assessment factors, are applied to the lowest of the available eco-toxicity figures and these factors depend on the availability of eco-toxicity data. The assessment factors that should be applied can be found in the TGD.

If the equilibrium partitioning method has been used to find the PNEC for sediment an additional factor of 10 has to be applied to the assessment factor.

Result: Predicted No Effect Concentrations (PNECs) for water, sediment and soil.

2.4 Determining the Risk Characterisation Ratios (RCRs)

6. The RCRs are calculated as the ratio between the PEC and the PNEC for each of the environmental compartments

Result: a table with all of the RCR figures for the different compartments and the release points.

If any of these RCR figures are higher than 1, further development of the model or more site specific measurements may be needed.

MINING APPLICATION

2.5 Introduction

This example describes a site specific, initial environmental risk assessment (ERA), which is based on site specific data and includes many hypothesis and scenarios.

The mining company wanted to start using a new flotation agent in order to extract mineral more efficiently and the company therefore needed permission from the authorities. The authorities requested information from the company on risks associated with the use of the chemical at the mining site. Data were therefore gathered and an initial risk assessment was conducted. This example is a further development of that risk assessment and focuses mainly on the risk to a river and the groundwater in the vicinity of the site.

The ERA points out risk hot spots and should be regarded as a basis for further work.

2.6 Background

2.6.1 *Chemical data*

The chemical is used to remove minerals.

Data on the chemical

- Molecular weight
- Molecular structure
- Water solubility
- Vapour pressure (20°C)
- pH
- Density (20°C)
- Biodegradability
- Eco-toxicity for two trophic levels

2.6.2 *Site description*

The mining site had been in operation for about thirty years before the introduction of the flotation agent in question. The layout of the site is illustrated below.

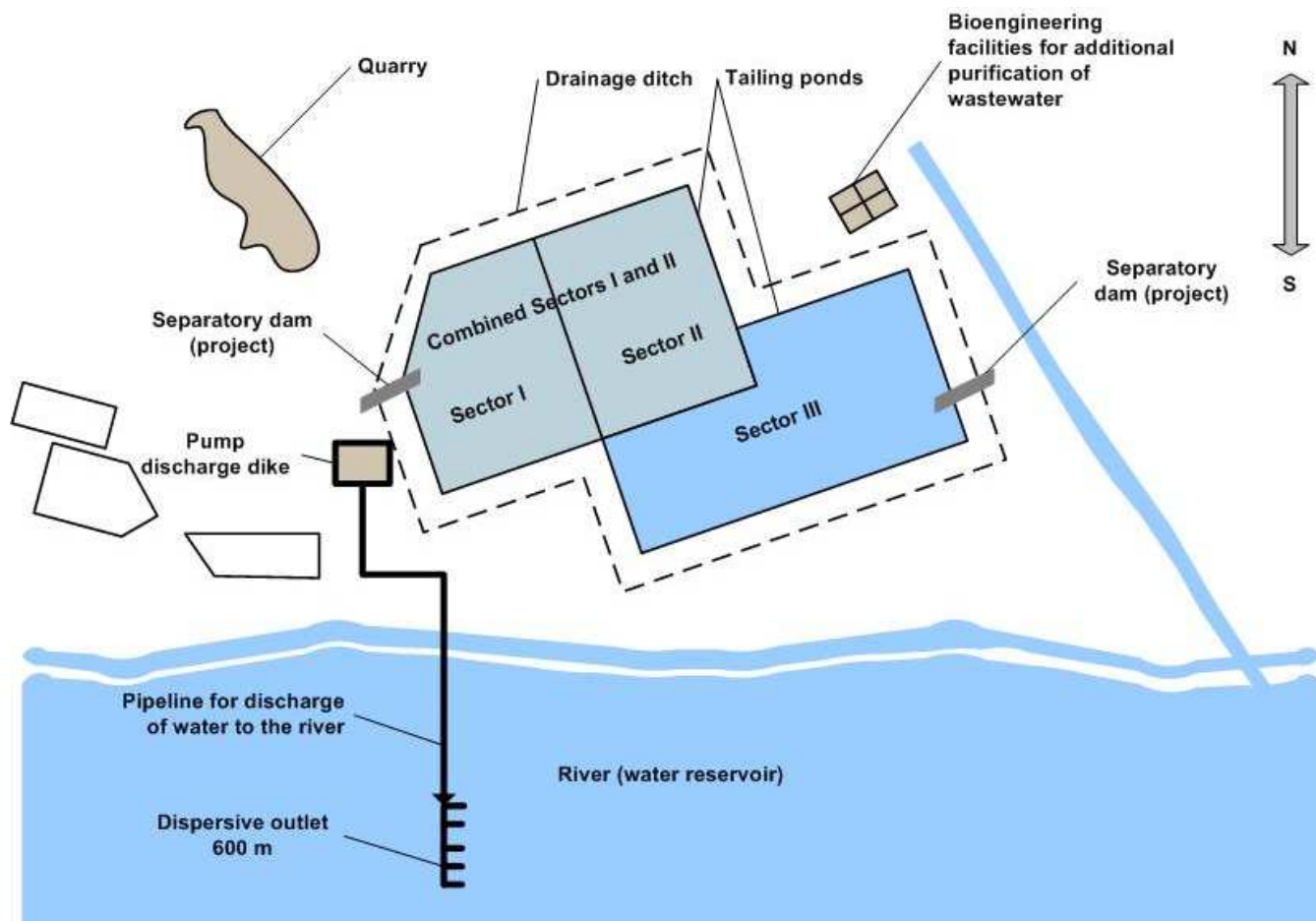


Figure 1. Overview of the tailing ponds

Due to the adsorptive nature of the flotation agent, a large fraction is adsorbed to the residual mineral surfaces during the flotation process. Residual mineral and chemicals (tailings) from the ore concentrator are pumped into a tailing pond where excessive water is either re-circulated to the plant or discharged into the river. Each Sector (see Figure 1) is divided into 8 smaller compartments where the tailings are dumped.

Water in the tailing ponds seeps through the dam embankment into the drainage ditch and is from there discharged into the river (water reservoir). The water also leaks to the soil beneath the ponds and possibly to the groundwater and is released into the air on dust particles. These releases may have an effect on the surrounding environment. The objective of the study was therefore to estimate the concentration of flotation agent in the surrounding environment (PEC), and compare these concentrations with the concentrations needed to produce detrimental effects on the eco-system (PNEC).

Site specific data

- Concentration of flotation agent in tailings water
- Adsorption onto tailings in the tailings water
- Water mass balance for the ponds including total and useable volume, water losses to fill the pores beneath the ponds and filtration losses that percolate through the embankment into the drainage ditch.
- Width, depth and minimum flow rate of the river

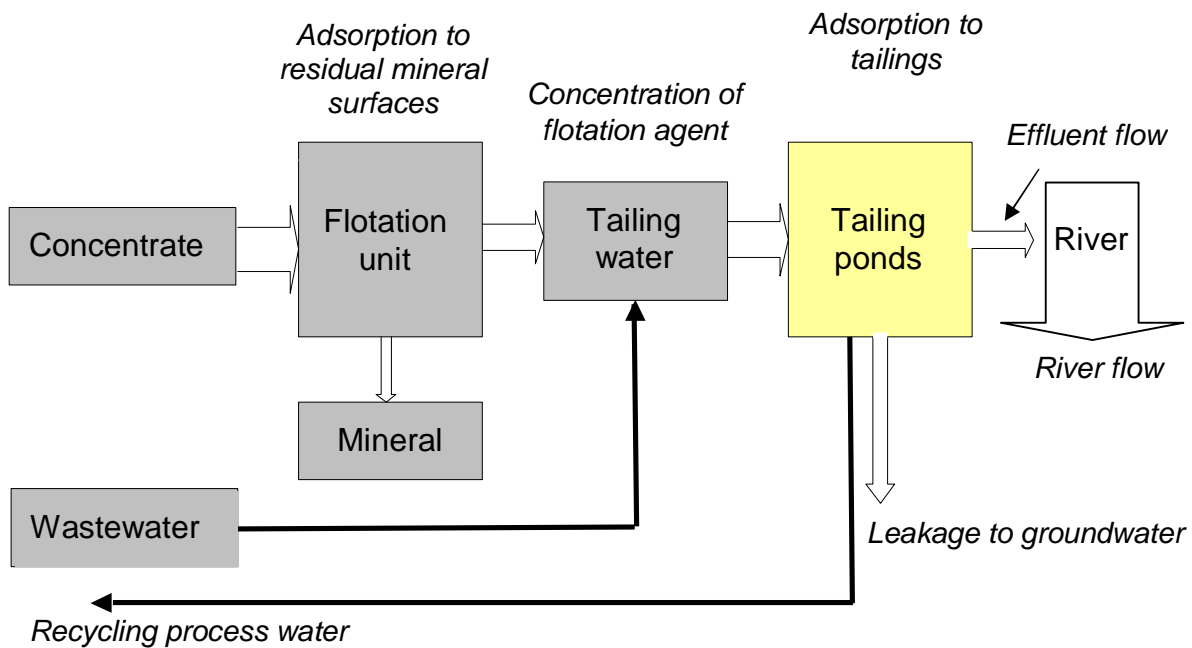


Figure 2. Flow diagram of water and flotation agent.

The incoming Concentrate and Wastewater comes from the primary and secondary separation processes and the Recycling process water is used in these processes.

2.7 Work and results

Firstly, the routes of chemical release had to be found. By looking at the layout of the site and the flows and mass balances, it was found that the chemical can be transported through the air on dust particles, seep through the old tailings in the ponds to the groundwater and seep through the embankment of the ponds into the drainage ditch and from there be pumped into the river.

2.7.1 Risk by inhalation

The site already had restrictions on the maximally allowed concentration of quartz in air. From this concentration and the concentration of flotation agent on solids in the tailings, the maximum concentration of flotation agent in air could be calculated. The maximum concentration of flotation agent was compared to Swedish threshold limits in air for quartz, beryllium dust and bensopyrene since no data on threshold limits allowed by the local authorities could be found.

No assessment of the risks to the surrounding soil and water catchments was made due to lack of data on the spreading of dust from the tailing ponds.

2.7.2 Risk to the groundwater

During the 30 years of use of these ponds, we assume that the water has percolated down and raised the ground water table to the level of the ponds themselves, i.e. the tailings are put directly into the groundwater. This results in a concentration in the groundwater equal to the concentration in the tailings water.

There were however no targets in the ponds of interest to protect and in order for the chemical to reach targets of interest to protect it would have to percolate through the old settled tailings on the bottom of the ponds and into the groundwater. From the area and total and useable volume of the ponds could be derived that the layer of old tailings was about 6.7 m thick beneath the water. From the water losses to fill the pores beneath the ponds and the area of the ponds the percolation velocity can be calculated. Degradation during the time it would take the water to percolate through the old tailings and into the groundwater were then considered by using chemical specific data on biodegradability and the default figures for degradation in soil from Table 8 in the Technical Guidance Document (TGD) [1].

There were two ways for us to find out how much of the chemical that will remain in the water phase and not be adsorbed to solids:

1. To use a measured figure for the fraction of chemical being adsorbed to solids, which was measured during a pilot plant study conducted at the mining site. The concentration in the tailings water (and groundwater) thereby decreases by this fraction.

2. The equilibrium partitioning method, which uses the sediment-water partition coefficient.

The local concentration in the groundwater (pore water) is then calculated as:

$$C_{\text{pore}} = C_{\text{pond}} * F_{\text{water}_{\text{sediment}}} / K_{\text{sediment-water}}$$

C_{pore}	concentration of chemical in pore water
C_{pond}	concentration of chemical in the tailings water
$F_{\text{water}_{\text{sediment}}}$	Fraction of water in sediment (default TGD, Table 3)
$K_{\text{sediment-water}}$	sediment-water partitioning coefficient

where

$$K_{\text{sediment-water}} = \frac{F_{\text{solid}_{\text{sediment}}} * K_{\text{p}_{\text{sediment}}} * \text{RHOSolid} + F_{\text{water}_{\text{sediment}}} + F_{\text{air}_{\text{sediment}}} * K_{\text{air-water}}}{K_{\text{air-water}}}$$

$F_{\text{solid}_{\text{sediment}}}$	Fraction of solids in sediment (default TGD, Table 3)
$K_{\text{p}_{\text{sediment}}}$	Solids-water partition coefficient in sediment
RHOSolid	Density of solid phase (default TGD, Table 3)
$F_{\text{water}_{\text{sediment}}}$	Fraction of water in sediment (default TGD, Table 3)
$F_{\text{air}_{\text{sediment}}}$	Fraction of air in sediment (default TGD, Table 3)
$K_{\text{air-water}}$	Air-water partition coefficient

Since $(F_{\text{solid}_{\text{sediment}}} * K_{\text{p}_{\text{sediment}}} * \text{RHOSolid}) \gg (F_{\text{water}_{\text{sediment}}} + F_{\text{air}_{\text{sediment}}} * K_{\text{air-water}})$ the result is

$$K_{\text{sediment-water}} = F_{\text{solid}_{\text{sediment}}} * K_{\text{p}_{\text{sediment}}} * \text{RHOSolid}$$

where

$$K_{\text{p}_{\text{sediment}}} = F_{\text{OC}_{\text{sediment}}} * K_{\text{OC}}$$

$F_{\text{OC}_{\text{sediment}}}$	Fraction of organic carbon in sediment (default TGD, Table 3)
K_{OC}	chemical specific partition coefficient between organic carbon and water (can be calculated as described in the TGD or with e.g. PCKOCWIN [3])

It has to be kept in mind that according to the TGD an additional assessment factor of 10 has to be applied to the sediment PNEC if the concentration in sediment or soil is calculated using the K_{OW} .

Concluding thoughts

The environment beneath the ponds is probably cold and dark and since the bottom of the ponds continuously is covered by mineral tailings with little organic material, the degradation may be very slow.

The percolation velocity and the concentration of the chemical should be measured in the groundwater and the flow of the groundwater should also be investigated.

2.7.3 Risk to the river

The tailings water percolates through the dam embankment and is pumped into the river through a pipeline with an unknown number of nozzles.

From the useable volume in the ponds and the filtration losses that percolate through the embankment the average dwell time of the chemical was calculated. During this dwell time the chemical is subject to degradation by using specific data on degradability and the default figures for degradation from Table 7 in the TGD.

During the percolation the chemical adsorbs to the soil in the embankment and the same calculations for adsorption as in the groundwater case above can be applied to this percolation.

A number of different scenarios can be applied to the release into the river. In this study we considered these:

1. Using the default dilution factor from the TGD for effluents being released into a river when no specific data are available. This default dilution factor is 10.
2. Total mixing, where the concentration in the effluent is diluted by mixing with the flow in the river. This resulted in a dilution factor of about 650.
3. Two computer programs for simulation of effluent discharges into river water, which can be found on the internet, were used to predict the concentration of chemical in the river. This scenario is described further below.

Using simulation software for river discharge

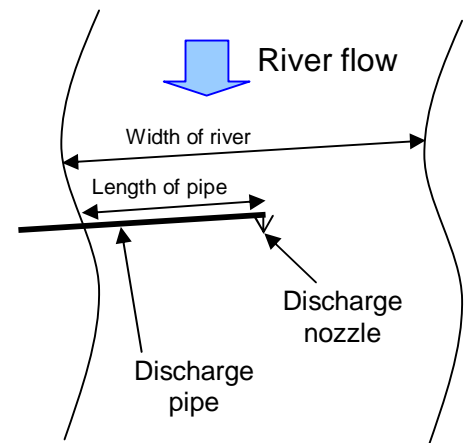
The two models included were the Rivmodel (from previous study) and the CORMIX-GI [2].

The Rivmodel showed a dilution factor of about 12 at a point 1000 m down river using one single discharge point.

Different cases were run with the CORMIX model, where the number of discharge nozzles and distances to and between the nozzles varied.

The dilution factor varied between 110 and 455 with 110 representing the most realistic scenario.

All of the data needed for the calculations could not be found and some figures had to be approximated.



As the chemical reaches the river water it will adsorb to suspended particles. The local concentration in the water is then calculated as:

$$C_{\text{water}} = C_{\text{river}} * F_{\text{water}}$$

C_{water}	dissolved concentration in water
C_{river}	concentration in river water
F_{water}	fraction of the chemical in the water phase

where

$$F_{\text{water}} = 1/(1+F_{\text{oc}} * K_{\text{oc}} * \text{SUSP})$$

F_{oc}	Fraction of organic carbon in sediment (default TGD, Table 3)
K_{oc}	chemical specific partition coefficient between organic carbon and water (can be calculated as described in the TGD or with e.g. PCKOCWIN)
SUSP	concentration of suspended matter, dry weight (default TGD, Table 3)

Concluding thoughts

In order to confirm the model, measurements of the concentration of chemical in the discharge pipe and 1000 m down river from the pipe could be conducted.

1.1.1 Effects assessment

From chemical specific eco-toxicity (e.g. LC_{50}) a Predicted No-Effect Concentration can be derived by applying assessment factors from the TGD (Table 16). In this case there were eco-toxicity data for only two trophic levels, which means that an application factor of 1000 was applied to the lowest eco-toxicity figure.

1.1.2 Risk characterisation

The Risk Characterisation Ratio (RCR) is calculated as the quotient of the exposure concentration and the effect concentration. If this ratio is above 1 further measures have to be taken to either reduce the predicted exposure concentration or to increase the predicted no-effect concentration. This can be done e.g. by making measurements as proposed in the concluding thoughts above or by making more eco-toxicity tests in order to reduce the assessment factor.

3 ASPHALT APPLICATION

3.1 Introduction

The scope of the study was to make a detailed analysis based on a previously made initial risk assessment of an adhesion promoter used in asphalt. The study was concentrated on the environmental releases during construction and use of a road and predictions of the environmental concentrations more in detail. The assessment was made in accordance with the EU Technical Guidance Documents (TGD) using the available data and default environmental parameters.

3.2 Background

3.2.1 Chemical data

The chemical is used to promote the adhesion between the aggregate and the bitumen.

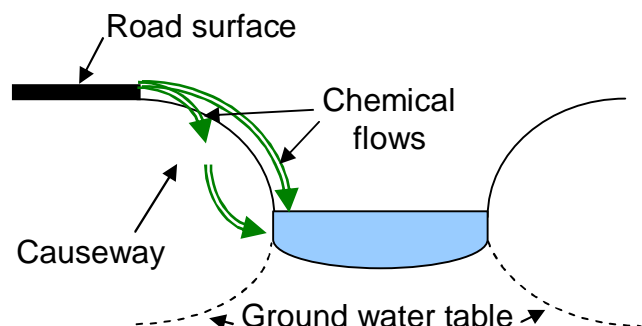
Data on the chemical

- Molecular weight
- Molecular structure
- Water solubility
- Vapour pressure (20°C)
- pH
- Density (20°C)
- Biodegradability
- Eco-toxicity for three trophic levels

3.2.2 Site description

The road that was considered was a Swedish country road and the size of the ditch was the default size from the TGD. The used parameters were:

- Width of road – 9 m
- Width of ditch – 2 m
- Water depth in ditch – 0.25 m
- Width of causeway – 0.5 m
- Depth of causeway – 0.5 m



3.3 Work and results

3.3.1 Effect assessment

The PNEC for aquatic organisms was derived from the lowest figure on acute toxicity. Since the available information about toxicity was for acute toxicity only the assessment factor is set to 1000, giving

$$\text{PNEC} = L(E)C_{50,\min} / 1000 \quad (1)$$

3.3.2 Construction

During or shortly after construction of the road, the chemical may be washed off the road surface by rain. The release during the construction of the road was assumed to be limited to the surroundings of the road. This is due to the low water solubility of the chemical and the high adsorption to soil.

The single dose of the chemical per meter of road that can be released, e.g. during rain, directly following an application of asphalt was calculated as:

$$\text{Dose} = F_{\text{comp}} * \text{rate} * (1 - F_{\text{ads}}) * \text{Width}_r \quad (2)$$

Dose	Single dose of chemical	
F_{comp}	Fraction chemical in emulsion	
Rate	Application rate of emulsion	
F_{ads}	Fraction of chemical adsorbed to the road	
Width_r	width of road	9 m

The water runs into the causeway where 25% of the chemical is adsorbed to the soil and 75% runs directly into the ditch (default TGD values). Using a partition equilibrium method derives the mass of the chemical in the pore water of the soil, which will percolate down into the ditch.

$$m_{\text{pore}} = \text{Dose} * F_{\text{inf}} * F_{\text{water}}_{\text{soil}} / K_{\text{soil-water}} \quad (3)$$

m_{pore}	mass of chemical in pore water	
F_{inf}	Fraction infiltrating into soil (default TGD)	0.25
$F_{\text{water}}_{\text{soil}}$	Fraction of water in soil (default TGD)	0.2 m ³ /m ³
$K_{\text{soil-water}}$	soil-water partitioning coefficient	

where

$$K_{\text{soil-water}} = F_{\text{solid}}_{\text{soil}} * K_{\text{p}}_{\text{soil}} * \text{RHOsolid} + F_{\text{water}}_{\text{soil}} + F_{\text{air}}_{\text{soil}} * K_{\text{air-water}}$$

$F_{\text{solid}}_{\text{soil}}$	Fraction of solids in soil (default TGD)	0.6 m ³ /m ³
$K_{\text{p}}_{\text{soil}}$	Solids-water partition coefficient in soil	
RHOsolid	Density of solid phase (default TGD)	2500 kg/m ³
$F_{\text{water}}_{\text{soil}}$	Fraction of water in soil (default TGD)	0.2 m ³ /m ³
$F_{\text{air}}_{\text{soil}}$	Fraction of air in soil (default TGD)	0.2 m ³ /m ³
$K_{\text{air-water}}$	Air-water partition coefficient	not calculated

In this case: $(F_{\text{solid}_{\text{soil}}} * K_{\text{p}_{\text{soil}}} * RHO_{\text{solid}}) \gg (F_{\text{water}_{\text{soil}}} + F_{\text{air}_{\text{soil}}} * K_{\text{air}_{\text{soil}}}) \Rightarrow$

$$K_{\text{soil-water}} = F_{\text{solid}_{\text{soil}}} * K_{\text{p}_{\text{soil}}} * RHO_{\text{solid}} \quad (3a)$$

where

$$K_{\text{p}_{\text{soil}}} = F_{\text{oc}_{\text{soil}}} * K_{\text{oc}} \quad (3b)$$

$F_{\text{oc}_{\text{soil}}}$ Fraction of organic carbon in soil (default TGD) 0.02 kg/kg
 K_{oc} Organic carbon-water partition coefficient

The mass of the chemical percolating through the soil into the water was very much less than the mass running directly into the water and we therefore neglected the percolating mass.

The peak concentration in the ditch following a road construction was therefore calculated as:

$$C_{\text{ditch,peak}} = \text{Dose} * (1 - F_{\text{inf}}) / (\text{Width}_{\text{water}} * \text{Depth}_{\text{water}}) \quad (4)$$

$C_{\text{ditch,peak}}$ peak concentration in ditch
Dose Single dose of chemical
 F_{inf} Fraction infiltrating into soil (default TGD) 0.25
 $\text{Width}_{\text{water}}$ width of receiving water in ditch (default TGD) 2 m
 $\text{Depth}_{\text{water}}$ depth of water in ditch (default TGD) 0.25 m

The concentration of the chemical to which aquatic organisms are exposed was calculated considering biodegradation and sorption to suspended organic matter in the water.

$$C_{\text{diss}} = C_{\text{ditch,peak}} * F_{\text{diss}} \quad (5)$$

C_{diss} dissolved concentration in water
 $C_{\text{ditch,peak}}$ peak concentration in ditch
 F_{diss} fraction of the chemical in the water phase

$$F_{\text{diss}} = 1 / (1 + F_{\text{oc,ditch}} * K_{\text{oc}} * \text{Susp}_{\text{ditch}}) \quad (5a)$$

$F_{\text{oc,ditch}}$ fraction org. carbon in suspended solids (default TGD) 0.1
 $\text{Susp}_{\text{ditch}}$ concentration suspended solids in a ditch (default TGD) 0.015 kg/m³
 K_{oc} organic carbon part. coefficient generated

K_{oc} can be measured by adsorption studies in for example OECD test guideline 106, but was calculated by PCKOCWIN [3] in this study.

The concentration in the ditch water for a certain time scale was calculated by taking biodegradation into account. The time scale is the one used for acute toxicity tests.

$$PEC_{\text{water,T}} = C_{\text{diss}} * 1 - e^{-k*T} / (k*T) \quad (6)$$

k rate const. for degr. surface waters (default TGD) 0.047 d⁻¹
 T time scale acute (default TGD) 4 d

The risk characterisation ration was then calculated as:

$$\mathbf{RCR_{water} = PEC_{water} / PNEC_{water}}$$

PEC_{water} Predicted Environmental Concentration
 PNEC_{water} Predicted No Effect Concentration

3.3.3 Use

When looking at the road over a longer period there is a possibility for leaching as well as abrasion of the asphalt. Leaching to the lower layers of the road under the asphalt is considered unlikely since the permeability of asphalt is very low. During the lifetime of the road the chemical will be released to the environment by abrasion of the asphalt. Abrasion depends mostly on the traffic load of the road and therefore differs considerably between different roads and places. According to literature [4] 5% of the released particles originate from bitumen, which corresponds roughly to the amount of bitumen added to the asphalt. It was assumed in this study that the release of chemical from abrasion is much larger than the release from leaching. A standard Swedish road wears about 0.2 mm per year across the road (except in the verge of approximately 1 m) and 0.5 mm in the worn tracks [5]. Estimating that 20% of the width of the road is the tracks, 0.8% of the road is worn off each year. We assumed a wear of 1% per year as a worst case. The particles from the road will probably spread some distance from the road, but as a worst case we assumed that all of the bitumen ends up just beside the road.

25% of the dose from the construction percolates into the causeway and forms an initial concentration in the soil.

$$\mathbf{C_{0,soil} = Dose * F_{inf} / (depth_{soil} * width_{soil} * RHO_{soil})} \quad (7)$$

C_{0,soil}	Initial concentration in soil	
Dose	Single dose of chemical	
F _{inf}	Fraction infiltrating soil (default TGD)	0.25
depth _{soil}	Depth in soil	0.5 m
width _{soil}	Width of soil	0.5 m
RHO _{soil}	Bulk density of soil (default TGD)	1700 kg/m ³

After the construction of the road it was assumed that the chemical is slowly released from the road to the causeway and ditch by abrasion and degraded in the process.

$$\mathbf{PEC_{soil} = D/k + [C_{0,soil} - D/k] * [1 - e^{-kT}] / (k * T)} \quad (8)$$

D	leaching flux from road to soil per day and kg soil	
k	rate constant for degradation in bulk soil (default TGD, table 8)	
T	averaging time evaluating soil ecosystem (TGD)	30 d

where

$$\mathbf{D = abrasion / (depth_{soil} * width_{soil} * Rho_{soil})} \quad (8a)$$

abrasion wear flux from road to soil

where

$$\text{abrasion} = F_{\text{comp}} * \text{Rate} * \text{Width}_r * F_w \quad (8b)$$

F_{comp}	Fraction of chemical in emulsion	
Rate	Application rate of emulsion	
Width_r	Width of road	9 m
F_w	Fraction of asphalt wear per day	$2.74 * 10^{-5}$ (1% per year)

In the absence of any eco-toxicological data for soil-dwelling organisms the $\text{PNEC}_{\text{soil}}$ may be calculated using the equilibrium partitioning method. This method uses the $\text{PNEC}_{\text{water}}$ for aquatic organisms and the soil-water partitioning coefficient.

$$\text{PNEC}_{\text{soil}} = K_{\text{soil-water}} * \text{PNEC}_{\text{water}} / RHO_{\text{soil}} \quad (9)$$

$K_{\text{soil-water}}$	soil-water partitioning coefficient
$\text{PNEC}_{\text{water}}$	Predicted no effect concentration

The equilibrium partitioning method does not consider the effects on soil organisms of chemicals that are adsorbed to soil particles and taken up by ingestion. When using the partitioning method for deriving $\text{PNEC}_{\text{soil}}$ for chemicals that have a $\log K_{\text{ow}} > 5$ an extra assessment factor of 10 is applied to the RCR according to the TGD.

The risk characterisation ratio for the causeway was therefore calculated as:

$$\text{RCR}_{\text{soil}} = \text{PEC}_{\text{soil}} / \text{PNEC}_{\text{soil}} * 10$$

The concentration in the ditch water is a sum of the amount of chemical in the pore water in soil and the amount running into the ditch on top of the soil. However, the amount running directly into the ditch is much larger than the percolating amount, which has therefore been neglected.

$$\text{C}_{\text{ditch}} = \text{Abrasion} * (1 - F_{\text{inf}}) / (\text{width}_{\text{water}} * \text{depth}_{\text{water}}) \quad (10)$$

The concentration of the chemical to which aquatic organisms are exposed is calculated considering sorption to suspended organic matter in the water and biodegradation.

$$\text{C}_{\text{diss}} = \text{C}_{\text{ditch}} * F_{\text{diss}} \quad (11)$$

C_{diss}	dissolved concentration in water
C_{ditch}	concentration in ditch
F_{diss}	fraction of the chemical in the water phase (see equation 5a above)

The concentration in ditch water for a certain time scale is calculated by taking biodegradation into account. The time scale is the one used for acute toxicity tests.

$$\text{C}_{\text{water,T}} = \text{C}_{\text{diss}} * 1 - e^{-k*T} / (k*T) \quad (12)$$

k	rate constant for degr. in surface waters (default TGD)	0.047 d^{-1}
T	time scale acute (default TGD)	4 d

As a worst case scenario it is assumed that the groundwater concentration is equal to the ditch water concentration, thereby neglecting dilution and transformations in deeper soil layers. The risk characterisation ratio is then calculated as:

$$\underline{RCR_{water} = PEC_{grw} / PNEC_{water}}$$

The concentration in the sediment of the ditch is calculated from the water concentration by applying the partition coefficient for the suspended matter in the ditch and water. An initial concentration from the construction of the road is also applied without any degradation.

$$PEC_{sed} = (K_{susp-water} / Rho_{susp}) * (PEC_{water} + C_{0,water}) \quad (13)$$

$K_{susp-water}$	Suspended matter-water partition coefficient	
Rho_{susp}	Bulk density of suspended matter (default)	1150 kg/m ³
PEC_{water}	Concentration in ditch water equal to PEC_{grw}	
$C_{0,water}$	Initial concentration in water equal to $C_{ditch,peak}$	

where

$$K_{susp-water} = F_{solid_{susp}} * K_{p_{susp}} * RHO_{solid} + F_{water_{susp}}$$

$F_{solid_{susp}}$	Fraction of solids in suspended matter (default TGD)	0.1 m ³ /m ³
$K_{p_{susp}}$	Solids-water part. coeff. in suspended matter	
RHO_{solid}	Bulk density of solid phase (default TGD)	2500 kg/m ³
$F_{water_{susp}}$	Fraction of water in suspended matter (default TGD)	0.9 m ³ /m ³

In this case: $(F_{solid_{susp}} * K_{p_{susp}} * RHO_{solid}) \gg F_{water_{susp}} \Rightarrow$

$$K_{susp-water} = F_{solid_{susp}} * K_{p_{susp}} * RHO_{solid} \quad (13a)$$

where

$$K_{p_{susp}} = F_{oc_{susp}} * K_{oc} \quad (13b)$$

$F_{oc_{susp}}$	Fraction of organic carbon in susp. matter (default)	0.1 kg/kg
K_{oc}	Organic carbon-water partition coefficient	

In the absence of any eco-toxicological data for sediment-dwelling organisms the $PNEC_{sed}$ may be calculated using the equilibrium partitioning method. This method uses the $PNEC$ for aquatic organisms and the sediment-water partitioning coefficient.

$$PNEC_{sed} = K_{susp-water} * PNEC_{water} / RHO_{susp} \quad (14)$$

When using the equilibrium partitioning method for deriving $PNEC_{sed}$ for chemicals that have a $\log Kow > 5$ an extra assessment factor of 10 is applied to the RCR .

$$\underline{RCR_{sed} = PEC_{sed} / PNEC_{sed} * 10}$$

3.3.4 Discussions and proposals

Leaching / abrasion

The RCR for the construction phase is proportional to the leaching from the road. It could therefore decrease the uncertainties to conduct further retention tests.

We have assumed that the chemical is released much more by abrasion than by leaching from the road due to the strong adsorption properties of the chemical. The assumed wear of the road of 1% may or may not be representative for e.g. a highway, but since the chemical is mostly applied to country roads, we believe this to be a good approximation. The RCRs for water and sediment for the use phase is almost proportional to the road wear.

Width of road

The chemical is mostly applied on country roads and therefore a width of about 9 m is used. All of the RCRs are proportional to the width of the road.

Infiltration into the roadside soil

The default fraction of rain water infiltrating soil is 25% in the TGD. Considering instead that all of the chemical is slowly infiltrating into the soil and only the mass in the pore water at equilibrium reaches the ditch water would increase the RCR for soil, but decrease all the other RCRs.

A slow infiltration of all of the chemical would possibly occur in road side soil that is made of gravel, which is fairly common.

Almost all of the chemical will consequently be adsorbed onto stone or bitumen particles as it is spread to the roadside. Since the chemical is adsorbed to particles it could be argued that more than 25% of the chemical will adsorb to or infiltrate into the soil since these particles sink.

One could also argue that the causeway is part of the road and not the environment, meaning that the chemical only poses a risk when it reaches the water in the ditch, thereby neglecting the concentration in the causeway soil.

An adsorption test for soil or gravel would be beneficial in order to know the amount ending up in the causeway and not in the water. Such tests and soils are described in the OECD Test Guideline 106.

Size of the road side soil

This aspect is hard to estimate and even though the volume of soil may be large, the chemical will most likely adsorb only to the absolute top layer of soil because of its' strong adhesion properties. This would imply that the concentration in the top soil layer is likely to be higher than estimated. One could however argue if a high concentration in the top soil layer of the road side poses a risk to the environment, since the road side does probably not constitute feeding grounds for any living organism, especially considering that a lot of other pollutants that end up by the road side (such as heavy metals, rubber, POCs and others). The RCR for soil is directly proportional to the width or depth of the road side soil. None of the other RCRs are affected. An adsorption test would ascertain how the chemical will be distributed between soil and water. Such tests and soils are described in the OECD Test Guideline 106.

Size of ditch

A default ditch is according to the TGD 2 m wide and 0.25 m deep. The width and depth have been halved in order to better fit Swedish conditions. Since the RCRs for water and sediment are proportional to the size of the ditch, using a default size ditch will decrease the RCRs for water and sediment by 75%.

Sediment toxicity

The high adsorption properties of the chemical result in a high concentration in the sediment as the road particles sink to the bottom of the ditch. The chemical will therefore not be biologically available to other organisms than possibly to those that eat the sediment. No degradation test for anaerobic conditions is available and therefore no degradation has been accounted for in the sediment.

Partitioning coefficients within actual range

All of the partition coefficients are based on a calculated value from PCKOCWIN, implying that the coefficients should be used with caution. We have however compared calculated values with measured ones [6] for a similar chemical and for this chemical the K_{oc} was fairly correct. All of the RCRs are almost proportional to K_{oc} . A standardized adsorption test would show more about how the chemical is distributed in the environment. Such tests and soils are described in the OECD Test Guideline 106.

4 HYPHENATIONS

PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
RCR	Risk Characterisation Ratio = PEC/PNEC
LC ₅₀	Lethal Concentration to 50% of exposed population
EC ₅₀	Effect Concentration detected in 50% of the exposed population
NOEC	No Observed Effect Concentration
t ₅₀	half life, time it takes for half of the chemical to degrade

5 REFERENCES

1. Technical Guidance Document on Risk Assessment for New and Existing Substances. <http://ecb.jrc.it/Technical-Guidance-Document/>.
2. CORMIX mixing zone model can be found at <http://www.cormix.info/>.
3. PCKOCWIN is part of the software EPISuite, which can be found at <http://www.epa.gov/oppt/exposure/docs/episuitedi.htm>.
4. Gustavsson, M. *Icke avgasrelaterade partiklar i vägmiljön* (in Swedish). Report from Väg- och transportforskningsinstitutet. 2001.
5. Personal communication with Bo Simonsson at Vägverket.
6. Slangen P.J. *Adsorption/desorption of octadecylamine on soil, sediment and sludge*. 2000.
7. EUSES (European Uniform System from the Evaluation of Substances) can be downloaded at <http://ecb.jrc.it/Euses/>.