



Environmental risk assessment of an adhesion promoter used in asphalt



Degree Project
in Engineering Chemistry
2002

Christina Berggren



Abstract

The aim of this thesis work was to carry out an Environmental Risk Assessment of a product, AA017, used as adhesion promoter in hot mix asphalt. AA017 is a development product from a product called Wetfix I. The product is produced by Akzo Nobel Surface Chemistry that has also initiated this work.

The Environmental Risk Assessment procedure is a way of evaluating the possible hazardous effects that a substance can have in the environment. This is done by estimating the concentration of the substance in three compartments, water, soil and sediment and comparing these concentrations with the sensitivity of these ecosystems. This means that the Predicted Environmental Concentrations (PECs) in different compartments are compared with the Predicted No Effect Concentrations (PNECs). A Risk Characterisation Ratio (RCR) is obtained by dividing the PEC with PNEC. If this ratio is higher than 1, the substance can constitute a risk in that compartment. The risks are evaluated for different compartments in different stages of the lifecycle of the substance.

The assessment performed in this work was done according to the Technical Guidance Document provided by the European Commission. Software called EUSES (European Union System for the Evaluation of Substances) has been used for some of the model calculations.

The emissions of AA017 differ for every stage of the product lifecycle. An emission scenario was created to map out the possible emissions and distribution routes during the lifecycle and compare with the model calculations.

The credibility of an Environmental Risk Assessment depends on the quality of the data that has been used in the calculations. Parameters like LC/EC50 for daphnia and melting point were adapted from a similar product and the vapour pressure was estimated. This is an important aspect to be aware of when looking at the final results. The results show no risks in the production and formulation stages and no risks on a regional level. In the processing stage the conclusion was that further information and/or tests are needed about the releases to be able to assess any possible risks during these stages. Further information and tests are also needed for the properties of the substance.

Preface

This report is a thesis work for the Master of Chemical Engineering program at the University of Umeå, Sweden. The work was carried out from January to August 2002 at Environmental Development at Akzo Nobel Surface Chemistry in Stenungsund, Sweden that also was the initiator of this thesis work.

The work has been very rewarding in terms of how much I have learnt, both about the subject of the thesis and about how environmental work is handled in large industries.

I wish to thank my supervisors at Akzo Nobel Klas Hallberg and Karin Sanne for enthusiastic guidance and help with both practical and theoretical issues. I would also like to thank my supervisor at Umeå University, Mats Tysklind and the Steering group at Akzo Nobel Jan Rosenblom and Bengt-Arne Thorstensson for ideas and advice during the work.

A special thanks to Marc Geurts at Akzo Nobel in Arnhem, Netherlands for helping me with the model calculations and a lot of other things.

Many thanks to Eva Nabseth Akzo Nobel for answering a lot of questions.

Finally, I would like to thank Sten Persson and his colleagues at Akzo Nobel Surface Chemistry in Stockvik, Sweden for a very rewarding visit at the factory and all the people at Environmental Development in Stenungsund for pleasant and well needed coffee breaks.

Christina Berggren

Stenungsund, September 2002

PREFACE	2
APPENDIX:	4
2. BACKGROUND INFORMATION	6
2.1 The product	6
2.2 The study.....	6
2.3 Comparison between LCA and ERA	6
2.4 Legislation and demands from the European Union	7
3. INDUSTRIAL ENVIRONMENTAL INFORMATICS	8
4. DESCRIPTION OF THE SUBSTANCE ASSESSED	9
Compound identification	9
5. MODEL DESCRIPTION - GENERAL.....	10
5.1 Input.....	10
5.2 Release estimation	10
5.3 Environmental distribution.....	11
5.4 Exposure assessment.....	11
5.5 Effect assessment.....	12
5.6 Risk characterisation	12
6. LIFECYCLE OF AA017 AS AN ADHESION PROMOTER.....	13
6.1 Production	13
6.1.1 Process.....	13
6.1.2 Treatment of the emissions.....	13
6.2 Formulation - Hot Mix.....	14
6.3 Processing - Asphalt pavement	14
6.3.1 In the road.....	14
6.4 Recovery of the road	14
7. OTHER APPLICATION AREAS FOR THE PRODUCT	15
7.1 Possible future application area for AA017/Wetfix I.....	16

8. EMISSION SCENARIO FOR EVERY STAGE OF THE LIFECYCLE	16
8.1 Production	16
8.2 Formulation	16
8.3 Processing	17
8.3.1 Construction of the road	17
8.3.2 Use of the road	17
8.4 Recovery.....	18
9. MODEL CALCULATIONS FOR THE RISK ASSESSMENT.....	19
9.1 Processing stage – Construction and use of the road	19
9.2 Model calculations for the risk assessment	19
10. TOTAL RESULT FOR ALL STAGES IN THE LIFECYCLE.....	20
11. ASSESSMENT OF SECONDARY POISONING.....	20
12. COMPETITORS	21
13. DISCUSSION	22
14. REFERENCES:.....	24

Appendix:

1: DATA USED IN THE MODEL CALCULATIONS IN EUSES

2: CALCULATIONS OF LOGKOW FROM KOWWIN

3: ANOTHER FRAMEWORK FOR ENVIRONMENTAL RISK ASSESSMENTS-US ENVIRONMENTAL PROTECTION AGENCY (EPA)

4: WARM RECOVERY OF ASPHALT

1. Introduction

An Environmental Risk Assessment (ERA) is a process of identifying and evaluating the adverse effects caused by chemical substances that may affect the environment.

ERA can be useful in many ways. One important aspect is that it provides a systematic procedure for reducing the risk that potential sources or mechanisms of pollution are overlooked. It can also show if measures are needed to limit the consequences that a substance can cause and it can point out if further testing and knowledge about a substance is needed.

The aim of this study is to collect information about a product, AA017, and then carry out an assessment of the environmental risks based on the Technical Guidance Document (TGD) provided by the European Commission. The substance assessed is the active substance in an asphalt product called AA017. This substance is used to improve the binding between the bitumen and stone material in asphalt. AA017 is a development product from a product called Wetfix I.

The producer of this product, Akzo Nobel Surface Chemistry has also initiated this thesis work. The decision to select AA017 as the product to assess was that Wetfix I had already been investigated from the perspective of a Life Cycle Analysis (LCA). These two studies will complement each other and form a good insight in the environmental impact of AA017/Wetfix I from two different points of views.

This report is the public report. More material is available for use within Akzo Nobel.

2. Background information

2.1 The product

AA017 is an adhesion promoter used in hot mix asphalt. It is a surface active product that improves the addition between the bitumen¹ and aggregate² surfaces and thus extends the life of the asphalt pavement. It is used in very small quantities in asphalt, only about 0.024% by weight. The active substance in the product is a tall oil fatty acid reaction product with polyethylene polyamines.

2.2 The study

The idea for Akzo Nobel Surface Chemistry is to learn more about the Environmental Risk Assessment procedure and investigate what information is needed for such a study and of course evaluate the results it gives for one particular product. The idea is to face the future demands the European Union will make for the chemical industry. These demands are for example increased information and registration about the properties of different substances. Further information about the EU demands can be given below, in chapter 2.4. The model calculations in this assessment are done using a program called EUSES 1.00 (European Union System of the Evaluation of Substances) [1]

The product Wetfix I that initially was decided for this study is going through modifications at the moment. The development product is made in higher temperatures and the structure of the active substance is slightly different. The active substance from the development product was assessed in this study according to its physico-chemical data but the production and sales figures were taken from Wetfix I. The emissions estimated from the production also originated from the production of Wetfix I.

2.3 Comparison between LCA and ERA

Even though the product assessed in this study is not exactly the same as in the LCA for Wetfix I it is worth comparing these studies since the use of AA017 will be the same as the use of Wetfix I. In combination, Life Cycle Assessment (LCA) and ERA form a very good insight into the environmental impact that an adhesion promoter can have.

The LCA shows the total emissions that are connected with the production and use of the product. The emissions originate from transports, energy use, pavement operations etc. The LCA also shows how much an adhesion promoter needs to extend the life of an asphalt pavement to yield a reduced environmental load of the pavement [2].

In the ERA the focus is only on the active substance in the product and the predicted releases to the environment and also the possible effects that the substance can have in different compartments are evaluated. In ERA no attention is paid to other emissions than those of the substance assessed. Thus both studies are needed to get a comprehensive picture of the environmental impact of a product.

¹ Bitumen is an oily material of low polarity with little chemical affinity for the aggregate

² Aggregate is the stone material used in asphalt.

2.4 Legislation and demands from the European Union

Last year (2001) the European Commission presented a White Paper-“Strategies for a Future Chemicals Policy”. The paper contains a proposed strategy for a new division of responsibility between industry, member States and the European Community. The intention is that the industry should be responsible for the safety of its products and the “burden of proof” to be shifted from authorities to industry [3]. The reason for this is to make the data collection and risk assessment processes more efficient and practical. Another reason for a new strategy is to get a better overview of all chemicals and thus also the risks [3].

A system called **REACH** (Registration, Evaluation, Authorisation of Chemicals) is created. This system will be used for assessing both new³ and existing⁴ chemicals and will contain the following elements:

Registration of basic information for all new and existing chemicals exceeding a production volume of 1 tonne per year. The information should be gathered in a central database. The registration should among other things include information about the intended use of the product and a preliminary risk assessment covering the intended uses [4].

Evaluation and assessment of registered information for substances with an annual production of more than 100 ton or for substances of concern. The producers will have to provide a risk assessment for the use of their products and a strategy for further testing. Then the Member State authorities will evaluate this strategy and decide on an appropriate course of action [4].

Authorisations include substances of very high concern. That is e.g. substances that are carcinogenic, mutagenic or substances that can cause disturbance in reproduction and persistent organic pollutants. Industries that wish to use this kind of substance for a particular purpose or as a component in a product must have a specific permission before such a substance can be used [4].

The REACH system will comprise about 30 000 different substances and it will exclude substances used in research and development [4]. An expanded European Chemical Bureau that could give technical and scientifically support should also administrate the REACH system [4].

Other features of the proposed system are, as mentioned before, that the responsibility for testing and risk assessments will be shifted from authorities to the industry. This includes also downstream users when the usage differs from those the manufacturer pictured. Importers will also need to carry out risk assessments [4]. Further, the White paper contains new strategies for chemicals in many other areas as well. During spring 2002 the Commission will create a proposal for a new set of legislation which is expected to be finished during summer 2002. After that the proposal must be studied by the European Parliament, which probably suggest some changes. The aim is that the new legislation should come into force during the period of this parliament [4].

³ “New” chemicals are chemicals marketed in the EU after 1981

⁴ “Existing” chemicals are chemicals marketed in the EU before 1981

3. Industrial environmental informatics

This section will briefly describe what kind of information that is needed for an environmental risk assessment and how this information can be found and dealt with. Further, it will discuss the problems that the gathering and evaluation of information can cause.

A list of the parameters that have been used for the model calculations in this environmental risk assessment can be seen in appendix 1. The parameters marked with * are necessary for a risk assessment in EUSES. Some of the physico-chemical parameters of the substance that are needed can be found in product safety data sheets. However, these sheets do not always contain sufficient information, e.g. the vapour pressure can be missing. In these cases it is necessary to search for information in other places, for example in databases that are supplied by different national environmental protection agencies. Different “experts” can be consulted about missing parameters and a value might be found for a reasonably similar product. Such “experts” can be for example the Research Manager responsible for the product. In some cases a Structural Analysis program, can calculate parameters such as the log Kow value. For ecotoxicological data the same problem can occur, that no information can be found in the safety data sheet and in different databases. A possibility can be to search for ecotoxicological-data for similar substances with similar structures. Of course expert judgement is needed in this case as well.

In an environmental risk assessment an important parameter is the volumes produced and sold. The usage of the substance must also be clarified since all areas where the product is used must be assessed. This kind of information can be supplied by the industry. The problem in this case is that the substance assessed can be mixed into different products in different amounts and it can be difficult to trace the substance. In big companies the products with the assessed substance might be sold under different names in different markets. Then it can be hard to know if all the usage areas and volumes are gathered. Another thing that causes problems is that the same substance can be known under several different names. In some cases the chemical name is used and in some cases some local abbreviations are used. The lack of uniformity can cause problems when communicating with different people.

When the production and use of a substance is limited to just one site and one usage it is wise to create an emission scenario for the particular product of interest. Information about emissions from a certain plant is of course supplied by the factory and sometimes in the environmental report. The emissions that can occur during the lifecycle of the substance can be estimated if detailed information about the fate of the substance can be gathered. Information like this can be found in the literature and by talking to people who work with the product. Expert judgements about sources of emissions are very useful as well.

4. Description of the substance assessed

Compound identification

Product name: AA017
CAS name: Fatty acids, tall oil, reaction products with polyethylenepolyamines
EINICS no: 272-756-1
Structural formula⁵:

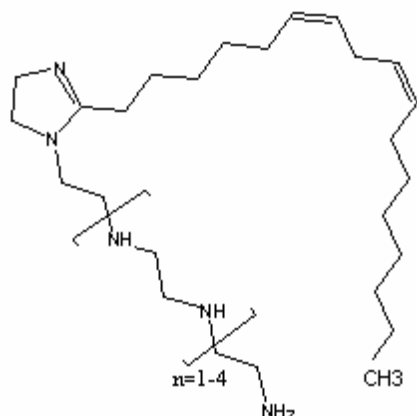


Figure 1: Structure of the substance

Molecular weight: 477-605 g/mol
LogK_{ow} = 4.2-5.7
Water solubility < 0.1 mg/l
Vapour pressure: 50 Pa
Melting point: -7 °C
Biodegradability: Inherently
Tox data: EC50 (48h) 0.49 mg/l, daphnia

Note: The LogKow is calculated with an estimation program called KOWWIN.
See appendix 2.

The measured tox data is from a test (OECD Guidelines 202) on Tall oil fatty acid reaction with tetraethylenepentamine. The melting point originates from the same substance as tox data. Due to the lack of measured data of the vapour pressure the value of the ethylene amines is used. It is considered as the most volatile of the primary products [5].
The biodegradability is assumed to be inherently as a worst case scenario since “not biodegradable” is not realistic in this case [5].

⁵ The structure can differ; the hydrocarbon chain that originates from the tall oil fatty acid can have more or fewer double bounds. The other chain can have various lengths, which explains the molecular weight interval. This structure can be seen as the most common one.

5. Model Description - General

This section is a brief description of the frameworks used in the European risk assessment system. The focus is on the environmental risk assessment on a local and regional scale and on existing substances. Detailed information for every module in the model can be found in the TGD and the EUSES user manual [1][6].

The structure of the system can be separated into different main modules as shown in figure 2

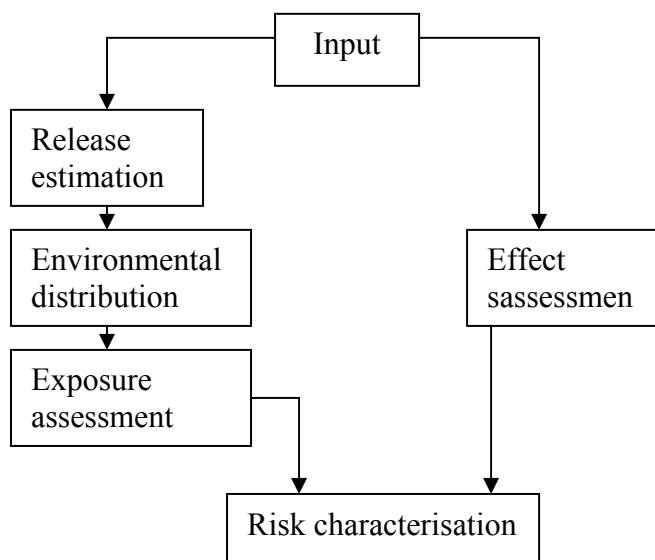


Figure 2. System structure

5.1 Input

In the input module there is a request for substance identification such as name, CAS-number and data on the physico-chemical properties [1]. The data that is available for new and existing chemicals is the “base set” as defined in a directive from the EU [3]. The availability of data differs depending on the type of substance that is evaluated. EUSES can work with very limited datasets. Other parameters that are needed in a risk assessment so-called secondary data such as partition coefficients and bio concentration factors will be estimated or set to default values. Missing data that can not be estimated should be set by a worst-case approach [1]. The quality of the data needs to be evaluated by the user of EUSES [1].

5.2 Release estimation

The release into the environment needs to be mapped for every stage in the lifecycle of the substance. The different stages are production, formulation, processing, private use and disposal [6].

The definitions for each stage are briefly as follows:

Production

The stage, in which the substance is manufactured, formed by chemical reactions, isolated, purified etc. [1].

Formulation

When the chemicals are combined in a process of blending and mixing to obtain a product or preparation. In this case, the step when the adhesion promoter is combined with bitumen and aggregate to form asphalt [1].

Processing

The process when the product or the formulation is used for example when a hot mix is paved on a road [1].

Private use

This stage can be considered if the substance is used by households and consumers [1].

Disposal

This stage considers disposal of the substance by waste or wastewater and recovery of the substance, or a product with the substance present. At the moment there are no quantitative methods in EUSES for estimating emissions at the disposal stage [1].

Release of a substance depends on the use pattern, three different types of use categories are distinguished in risk assessments: main category (MC), industrial category (IC) and use category (UC) [6].

The MC gives a general description of the exposure relevance of the substance and it describes a rough release scenario during the production, formulation and processing stages. The IC specifies to the sort of industry where considerable emissions occur during the application of the substance. Each IC provides release tables for the different stages of the lifecycle. These release tables are used as default values when no other information is available and they can be considered as very general. The default values in EUSES are generally very restrictive. Any relevant information can be used to override these default values [1].

The UC describes the function of the substance. There are many examples of use categories and they have varied levels of details. There are tables in the TGD that can be useful when deciding which use category to choose. Some of the use categories have specific scenario documents available. Specific information about a substance from a producer or similar is even more relevant [6].

5.3 Environmental distribution

The distribution of a substance in the environment is assessed on two spatial scales, a local scale, close to a point source and a regional scale including both point and diffuse sources. The local scale is considered as an area with a radius of 1km around the source. The size of the regional standard environment is 200*200 km. The regional area is considered to be a standardised European area regarding population and other parameters [1]. The fate of the substance released is estimated by considering routes of exposure and biotic/abiotic transformation processes. The secondary data such as partitioning coefficients, bio-concentration-factors and degradation rate constants are derived from the primary data of the input module [1].

The quantification of the distribution and the degradation of the substance lead to an estimate of the Predicted Environmental Concentrations (PECs) on a local and regional scale. In most cases the regional PEC provides a background concentration for the calculation of the local PEC [1].

5.4 Exposure assessment

The exposure assessment deals with secondary poisoning. Exposure levels for humans and predating birds and mammals are estimated.

The concentration in food of higher organisms is estimated from the concentration in the environment and by looking at different food chains. Bioconcentration and bioaccumulation is an important aspect for lipophilic organic chemicals and some metal compounds [6].

5.5 Effect assessment

In this part of the assessment toxicological data is needed. It is used for the dose/concentration – response/effect assessment and to determine the Predicted No Effect Concentration (PNEC). A PNEC value can be derived for microorganisms in STPs, aquatic organisms (algae, daphnia and fish), terrestrial organisms, birds and mammals. These represent ecosystems that are all considered as environmental protection goals.

A PNEC is regarded as the concentration below which an unacceptable effect will most likely not occur. The PNEC is calculated by dividing the lowest short term LC50/EC50 or long term NOEC by an appropriate assessment factor. This factor shows the degree of uncertainty when extrapolating the laboratory toxicity data to a complex environment. The assessment factors vary from 10 to 1000 depending on how much information is available. For example only one short-term LC50/EC50 for fish give the highest assessment factor. The assessment factor can be varied under certain circumstances. Some important assumptions that have been made for the aquatic environment are that the ecosystem sensitivity depends on the most sensitive species and that protection of the ecosystem structure protects community function [1][6].

5.6 Risk characterisation

A risk characterisation ratio (RCR) is calculated for each chemical life-cycle stage and for each end-point (assessed organisms). The RCR is obtained by dividing PEC by PNEC. This comparison between the toxic effects and the estimated concentrations are a central idea in the environmental risk assessment procedure.

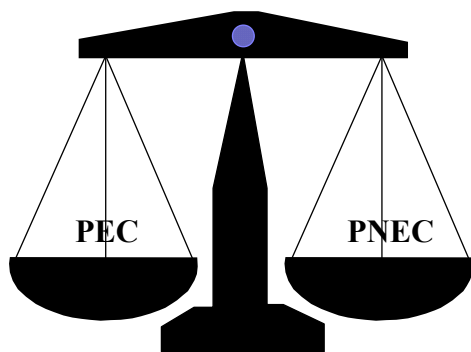


Figure 3: Illustration of the risk characterisation procedure, the PEC and the PNEC are compared.

The conclusions that can be drawn from the RCR values depend on whether it is a new or existing substance that is characterised and there are different strategies to follow when the RCR is bigger than one. The general procedure for the risk characterisation according to the TGD is as follows:

- Determining the RCR for the different protection goals and depending on this:
- Determining if further information/testing can lead to a revision of these ratios
- Asking for further information/testing when appropriate
- Refining of the RCR.

This model for Environmental Risk Assessment is used in the European Union. There are other models for Environmental Risk Assessments in for example The United States. Further reading about the Risk Assessment procedure in the US can be found in appendix 3.

6. Lifecycle of AA017 as an adhesion promoter

6.1 Production

Since AA017 has not been produced in large scales facts about the production are taken from the production of Wetfix I. Being very similar products the later conclusions about the production are also relevant for AA017

6.1.1 Process

Wetfix I is produced in Akzo Nobel Surface Chemistry plant in Stockvik, Sweden. First the TOFA (Tall Oil Fatty Acids) and VEA (Various Ethylene Polyamines) are mixed in a reactor. The TOFA is added through a closed system from a tank and the VEA is pumped in from small containers. A venting system creates a vacuum in the reactor.

The water that is formed during the reaction leaves the reactor through a scrubber system [7]. A solvent is added to the cooled Wetfix IC and this blend is called Wetfix I. Wetfix I is made batch wise. After the process the reactor is flushed once with IPA (IsoPropyl alcohol), nitrogen and water. The flush liquid is then incinerated [7].

6.1.2 Treatment of the emissions

During the process, the air emissions go through an “acid scrubber” with sulphuric acid and the water from the scrubber is sent to a water treatment plant (WTP) via the same system as the other four scrubbers in the plant. It takes about 2 h for this water to reach the water treatment plant. [8] It treats the water in several steps by mechanical separation, chemical treatment and biological treatment with aerobic degradation [8].

The water treatment plant also receives surface water from the whole plant area. The recipient is the Gulf of Bothnia [9].

The flush water is sent to incineration that takes place at about 1000°C. Emissions from the incineration go through a venturi scrubber [7].

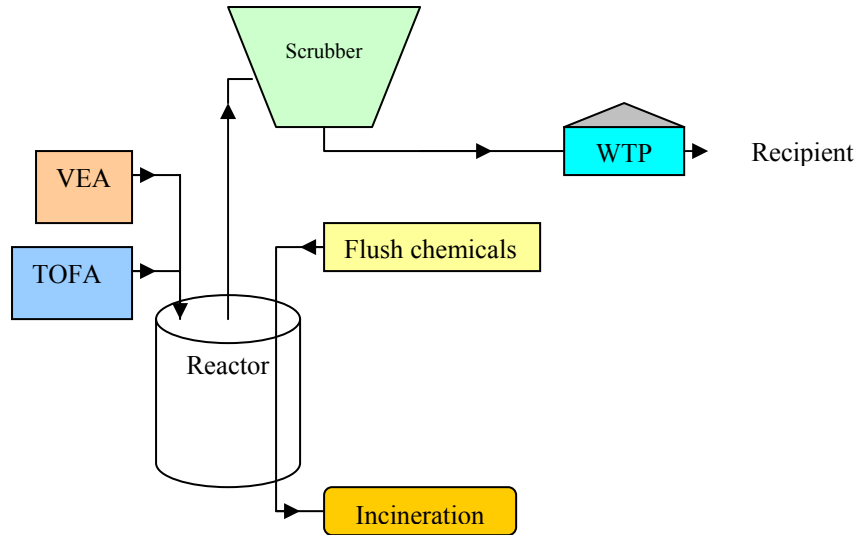


Figure 4. Wetfix I production-process description relevant also for AA017

6.2 Formulation - Hot Mix

AA017 is mixed with bitumen and aggregate to form asphalt. The amount is about 0.25-0.5% per weight of bitumen which is about 6 % of the weight of the asphalt [2]. AA017 and bitumen are mixed together in an asphalt work, which can be a big stationary work or a small mobile work situated near the road construction [10]. In 90% of the cases AA017 is added to the bitumen through a closed system. In the rest of the cases AA017 is added manually with buckets or pumps to the bitumen tank [10].

6.3 Processing - Asphalt pavement

To construct **1 km x 13 m** of a road (This unit were used in the LCA of Wetfix I and also in other LCA studies of roads) two layers of 1235 ton each of hot mix is needed. (This amount can differ considerably but these figures were also used in the LCA of Wetfix I and are considered for an average Swedish countryside road) Each ton of hot mix contains 240 g of AA017 (0.4 % per weight of bitumen)[2]. When the asphalt is paved it has a temperature of 150°-170°C [11].

6.3.1 In the road

During the lifetime of the road, which is considered to be 40 years, maintenance operations are done 3 times, each time a layer of 1235 ton.[2]

6.4 Recovery of the road

The recovery process can be separated into different steps:

- Removal and shaping
- Storing
- Recovery by different methods
- Pavement

Digging or cutting removes the asphalt layer. It is then separated from other materials and impurities like soil and clay and crushed to asphalt granulate. The removed asphalt sometimes

needs to be stored for a while. It can either be stored at permanent sites or temporary sites for example nearby an asphalt work. The storage time can vary considerably in Sweden it can be up to 3 years [12].

The recovery can be done in situ or in an asphalt work by three different methods, cold, medium warm or warm recovery. The process temperatures are in each case, <50°C, 50-120°C and >120°C. In all processes the recovered asphalt is mixed with new material such as bitumen, emulsions of bitumen, foam of bitumen and new asphalt material. When using medium warm and warm recovery adhesion promoters such as AA017 can be added. The proportion of recovered asphalt versus new material differs in every process [12]. When using the in situ recovery a special machine does cutting, mixing and pavement in one stage so there is no need for storing in that case.

The occurrence of the three main categories, cold, medium warm and warm recovery differs. In 1998 cold recovery was used for about 50% of the recovered asphalt, medium warm and warm for about 25% each. The choice of method depends partly on the traffic situation of the road and the local climate [11][12]. Some asphalt can not be recovered because of impurities and bad quality. In those cases it is put into landfills [11]. The amount of recovered asphalt in Sweden is unknown. Different parties such as the National Road Administration, different companies and municipalities take care of the recovery and consequently it is not possible to obtain an exact figure of the amount recovered asphalt [11]. Last year (2001) the figures for the National Road Administration (NRA) were as follows:

Recovery of asphalt mix	%	ton
Landfill	2.9	26 452
Used in new asphalt	63.7	589 540
Stored	14.5	134 585
Other ⁶	18.9	174 698
	100.0	925 275

The Swedish National Road Administration is required to recover 90% of new asphalt in the future [11].

More details about the warm recovery techniques can be found in appendix 4. The warm recovery is chosen for a further description since this technique gives the highest releases of adhesion promoters.

7. Other application areas for the product

There are other application areas for Wetfix I than the asphalt application. These application areas are either in very small amounts outside Europe or at a research stage and therefore these areas are just mentioned but not considered in the environmental risk assessment models [13].

⁶ Other usage is in most cases asphalt that has been milled with a cutter and used in the roadbed

7.1 Possible future application area for AA017/Wetfix I

At the moment, Wetfix I, AA017 and Wetfix IC are tested within other application areas as well. The purpose for this work is to replace non-environmental friendly products/chemicals with this chemistry instead.

The tests are carried out in cooperation with the customers. Tests are performed both in lab scale and in full scale before any decisions can be made about the usage of AA017. Which toxicological and ecotoxicological tests that will be done is according to the customers demands. It is very likely that the regulations within this new application area will call for more toxicological tests in the future.

Before it is possible to decide anything about using AA017 the customers must evaluate the technical function of the product and the toxicological tests [14].

8. Emission scenario for every stage of the lifecycle

This section describes the possible emissions that can occur during every stage of the lifecycle of an adhesion promoter. It is quite difficult to create an emission scenario for a product like AA017. No real measurements of possible emissions of this particular substance are done during any stage of the lifecycle. But with knowledge of the substance and the handling and use of it, it is possible to estimate theoretically the possible releases of the substance. This emission scenario is based on arguments, estimations and facts received from “experts” in different stages. Such experts are for example the Research Manager of the product, Bengt-Arne Thorstensson, people working with the emission control at the Stockvik plant and Bo Simonsson at the Swedish National Road administration. This theoretical discussion about releases is a complement to the later calculations in the risk assessment section.

8.1 Production

The emissions of the pure substance that can occur during the production stage can be considered to be limited. During the reaction the reactor loses 6 % of the weight but this is mostly water and some short amines from the VEA. [15] After the reactor, the emissions pass through a scrubber system and the water from that is treated in a water treatment plant. The efficiency in the biological treatment step is about 70 – 75 % so the total efficiency of the water treatment plant is even higher [9]. Almost all emissions from the production stage can be connected to the effluent water from the water treatment plant. The recipient from the water treatment is the Gulf of Bothnia. The outlet from the WTP is located about 100m out in the stream of the river Ljungan that flows out into the sea near the factory. The average flow of the river is $76 \text{ m}^3/\text{s} = 8294400 \text{ m}^3/\text{day}$. The average flow from the WTP is $460 \text{ m}^3/\text{day}$ [16]. This makes a dilution factor of about 18000.

8.2 Formulation

Emissions from this stage are very hard to estimate and model since the mixing between adhesion promoter, bitumen and granulate can be done in so many different ways and the possible emissions are very diffuse. The direct emissions to water in this stage are negligible [5] but there is a possibility of a release to air during the mixing process, especially when the adhesion promoter is added manually to the hot mix. The mixing process takes place at high temperatures and therefore the adhesion promoter could evaporate to the air. There is also

always a possibility of spillage to soil during the mixing. The leaching that could take place if the hot mix is stored on the ground before paving. However, this potential leaching is probably very limited due to the short time of this event.

8.3 Processing

During the processing stage, which in this case is the construction and use of the road, there is an emission peak when the asphalt is paved.[17] Since the temperature of the asphalt is about 150-170° C some of the product can evaporate from the road. Evaporation tests on the pure AA017 show that at 180° C about 3.2 % of the product disappears after 2 h [18]. In reality when the product is mixed together with bitumen and aggregate the amount that evaporates is much smaller. [5]

8.3.1 Construction of the road

The release during the construction of roads is probably limited to the surroundings of the road. This is due to the low water solubility and the high adsorption of the substance to the soil.[17]

8.3.2 Use of the road

When looking at the road over a longer period there is a possibility for leaching of the asphalt. Leaching to the lower layers of the road under the asphalt is most unlikely since the permeability of asphalt is very low. [11] If any leaching of AA017 takes place it will probably flow to the roadside. No specific studies on leaching of adhesion promoters from asphalt have been done so it is difficult to estimate a scenario. Leaching tests performed at the University of Florida came to the conclusion that there was no leaching of organic compounds from reclaimed asphalt pavement.[19] When considering this and the fact that AA017 is a surface active substance that binds very hard to any surface the leaching of AA017 from the asphalt is very limited.

A first rain scenario for a road building application has been done on an emulsifier called Duomeen T. In this test no Duomeen T was detected in the rain run off water. With a detection limit of 0.250 ppm it means that in this case 99.988% was adsorbed to the road. Since AA017 binds roughly as hard as Duomeen T to the asphalt [5] one conclusion for AA017 can be that at least 99.988% is adsorbed to the road during the first rain.

During the lifetime of the road there is a possibility that AA017 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. Every year about 110000-ton road surfacing is rubbed off in Sweden.[20] The released particles originate mostly from the aggregate but 5% originate from the bitumen, which corresponds to the amount of bitumen added to the asphalt.[20] Hence it is likely that some AA017 is released in this way, probably connected to a particle. This release is also probably limited to the surroundings of the road, about 50 m. It is hard to create a model and do calculations on this scenario but it is still an important aspect to be aware of.

Even though AA017 can adsorb easily to soil particles the sorption can vary a lot depending on the texture of the soil. In a soil made mostly of clay a higher degree of sorption will take place. Also the pH in the environment can affect the sorption since it affects the solubility of a substance. [21]

8.4 Recovery

The emissions of adhesion promoters that can occur during the recovery of the road are similar to those in the formulation step. The possible releases are diffuse and mostly to air. Emissions can occur both when the asphalt is cut up and when it is mixed with new asphalt in a work or in situ. An important aspect of the recovery stage is that the crushed old asphalt is sometimes stored for up to 3 years before it is recovered. During this time there is a risk for leaching of adhesion promoters and this risk is much higher than leaching from the road since the asphalt in this case is crushed. [11] Another critical part is the recovered asphalt that is used in the roadbed.

9. Model calculations for the risk assessment

9.1 Processing stage – Construction and use of the road

In this case the processing stage can not be calculated using the EUSES program. The Processing stage needs to be calculated by hand using another model. Such a model can be the Dutch USES model “run off to small surface waters”.

9.2 Model calculations for the risk assessment

Calculations in EUSES with refinements

The production and formulation stages in the lifecycle are calculated using the EUSES program this include also calculations on a regional level. The input data used in EUSES can be seen in Appendix 3. Some changes in the default settings of the program have been made when there is information available.

Changes in default settings of EUSES:

- No application of STP-sludge on agricultural soil and grassland
The only stage when sludge is produced is in the production stage and this sludge is not applied on agricultural soil so that kind of release can be excluded [8].
- The number of emission days in the production stage was changed to 19 d, which is the number of days that the chemical was, produced [7].
- The dilution factor after the WTP in the production stage was changed to 18000 after the calculation of the dilution from the river Ljungan [16]
- No emissions to waste water in the formulation step. This is because in the asphalt work no emission to waste water takes place [5].
- Assessment factor of 10000 for aquatic organisms instead of 1000 which is the highest default factor. This is a very protective assessment factor and is used since there is only one toxicological endpoint available. The daphnia is normally not as sensitive as algae [17].

With these changes in the default settings in the program the Predicted Environmental Concentrations (PECs) were estimated:

	PECwater (mg/l)	PECsoil (mg/kg)	PECsed (mg/kg)
Production	3.8E-05	4.7E-07	2.66E-03
Formulation	3.58E-07	5.24E-07	2.5E-05
Regional	3.58E-07	2.47E-09	3.74E-05

From these PECs the Risk Characterisation Ratios (RCRs) were decided: $PEC/PNEC = RCR$

	RCRwater	RCRsoil	RCRsed
Production	0.776	1.35E-04	0.878
Formulation	7.3E-03	1.5E-08	8.3E-03
Regional	7.3E-03	7.4E-06	0.0123

10. Total result for all stages in the lifecycle

Table 1: RCR for every stage of the lifecycle

Scenario	RCRwater	RCRsoil	RCRsed
Production	0.8	1E-04	0.9
Formulation	7E-03	2E-08	8E-03
Processing construction	Not enough data	Not enough data	Not enough data
Processing use	Not enough data	Not enough data	Not enough data
Regional	7E-03	7E-06	0.01

The RCRs are lower than 1 and thus does not indicate any risk.

11. Assessment of secondary poisoning

In the Technical Guidance Document (TGD) there is a part that deals with secondary poisoning. This section describes the properties of a substance that can indicate a risk for secondary poisoning. This is not considered in the risk characterisation but is an important aspect when looking at the total impact of the substance.

For lipophilic organic chemicals bioconcentration and bioaccumulation may be of concern. Bioconcentration is an increase in concentration of a chemical in an organism resulting from tissue adsorption levels exceeding the rate of metabolism and excretion. Bioconcentration deals with water borne exposure only. Bioaccumulation considers all routes of exposure such as food and environment. Biomagnification is accumulation of chemicals through the food chain that can give an increase at higher levels in the trophic chain [6]. One indication of bioaccumulation potential is a high value of the octanol-water coefficient. It is accepted that values of logKow greater than 3 indicate that a substance can bioaccumulate but for a surface-active substances this indication is uncertain [6]. Also adsorption onto biological surfaces such as gills can lead to bioconcentration. Thus a high adsorptive capacity can indicate potential of bioaccumulation [6]. Other things that can influence the bioaccumulation are the degradation rate and the molecular mass. A substance with a molecular mass above 700 can usually not be taken up by fish because of the steric hindrance at the cell membrane [6].

One way of assessing the risks for bioaccumulation is to measure the bioconcentration factor (BCF). This is the ratio between the concentration in the organism (mg/kg) and the concentration in the surrounding water (mg/l) at steady state [6].

In this case the calculations in EUSES suggest a BCF for fish around 700 l/kg which indicates that the substance has a moderate tendency to bioaccumulate[17] BCF values between 100 and 1000 mean that the substance can be classified to have moderate tendencies to bioaccumulate [6]. With this information in mind and when looking at the properties of the substance, $\log K_{ow} > 3$ and adsorptive, the conclusion is that AA017 can have a bioaccumulation potential.

12. Competitors

It is important to be aware that there might be other companies that produce the same or similar kind of substance as the one assessed in this report. If a similar product is produced and used in other parts of Europe this can affect the background concentration and thus the risk assessment on the regional scale. CECABASE has a product used as adhesion promoter that consists of amidoamines and imidazolines. There is a possibility that this is the same kind of substance as in AA017 and this could affect the concentration on the regional level. Considering the share of the market that Akzo Nobel has for adhesive additives it differs from about 100% in the Nordic countries to about 40% in Western Europe. This indicates that in the Nordic countries the use of a similar substance in asphalt is very unlikely [23].

13. Discussion

An environmental risk assessment is a complex way of evaluating the environmental load and impact of a substance. Many different parameters interact with each other to decide the distribution of a compound in the environment and finally estimate a PEC. This means that many of the parameters used in the model are very decisive for the final result. For example, all partitioning constants that are calculated based on the primary input data play a very important role in the distribution of the substance. Thus it is important to realize that the quality and credibility of the risk assessment is very dependent on the quality of the data used. Further, the amount of data plays an important role; the number of toxicological data will affect the effect assessment since the assessment factor depends on how many toxicological tests that are available.

Another thing that is important to notice is that the model calculations in the program EUSES are very general. A general, average European environment is defined and used in the calculations and general release tables are used in the cases where no other information is available. Therefore the results from the modeling can not be considered as some definite truth. Still in many cases they provide an idea about in what systems and lifecycle stages that the substance can constitute a risk. Emission sources that have not been noticed before can also be brought to light in this way.

An important aspect when discussing the result of this study is the fact that almost all parameters are either taken from similar products, calculated or estimated and this affects the credibility of this study. The PNEC is based on only one toxicological data from a substance similar to AA017 and thus there are some uncertainties in this PNEC. The very restrictive assessment factor of 10 000 will however most likely assure that the risks are not underestimated.

The conclusion from the processing stage is that it is not possible to exclude that construction and use of road can signify a risk. Another conclusion is that more knowledge about the releases and distribution of adhesion promoters near by roads and pavement areas is needed.

In the formulation stage there are no indications of any risks which correspond to the discussion in the emission scenario and thus the emissions of adhesion promoters at asphalt works are probably very small.

In the production stage the high dilution factor affect the result which shows no risk in any of the stages. The highest concentrations seem to be in the water and thus in sediment. This result also corresponds to the previous argument in the emission scenario.

The assessment for the regional scale shows that there are no risks on that scale and this is very likely since this substance is not so widely used and the amount produced is relatively small.

The bioaccumulation potential of this substance can not be excluded because of the properties of the substance for example the logKow value indicate a bioaccumulation potential. This indication is however not so reliable for surface active substances according to the Technical Guidance Document. The BCF calculated from EUSES suggests that the substance has a moderate tendency for bioaccumulation in fish. Since bioaccumulation is a very complex phenomenon some testing or measurements are needed to be able to say anything for certain.

To sum up the results from the risk assessment calculations the only stage in the lifecycle that seems to be of concern is the processing stage, since no emission data at all is available. The conclusions are thus that on the regional scale and in the production and formulation stage there is no need for further testing or information. For the processing stage the conclusion is that there is a need for further testing and information. These conclusions are based on the data available at the moment.

The information that is needed is how much AA017 leaching out during the use of the road. This can be obtained from a long term leaching study on asphalt. It is also necessary to investigate what emissions of AA017 that can occur during the road construction. It must be made clear if AA017 can evaporate from warm asphalt or not. A first rain scenario on warm asphalt is also an important investigation. It can be used to find out what concentrations AA017 can have in adjacent ditches if it rains during or after the pavement of asphalt. Another thing that is necessary to know is the bioavailability of if the substance associated to particles. This is important when considering abrasion of asphalt and the particles that are spread to the surroundings of the road due to it.

Other tests that are relevant are of course additional toxicological tests. Acute tests on algae, daphnia and fish and long term test on one trophic level would increase the credibility of a study like this. It would also most likely lower the risk ratios since the suggested tests would justify an assessment factor of 100 instead of 10000.

To facilitate this kind of work it would be desirable to have a database or equal sources of data where all this information is gathered in one place. In such system the quality of the data should be clarified or guaranteed. This means for example that if a parameter is estimated from a similar product, information about how the estimation is done, and by who should be supplied, so that the user of the data can judge if the parameter is relevant or not. This is important since, as mentioned before, in a study such as an environmental risk assessment the quality of the data used is very important and many of the parameters are critical for the final result.

14. References:

1. TSA group; European Uniform System of the Evaluation of Substances 1.00 user manual; Feb.1997
2. Ries Adeline; *Life Cycle Assessment of an adhesion promoter used in hot mix for asphalt pavement*; Master of Science thesis at Akzo Nobel; Chalmers University; 2001
3. Anita Ringström; *EU Kemikalie kontroll-REACH systemet*; Meddelandet Nr 11/2001
4. Commission of the European Communities; *White paper Strategy for a future Chemicals Policy*; February 2001
5. Personal communication with Bengt-Arne Thorstensson; Research Manager, Akzo Nobel Surface Chemistry AB; 2002
6. European Commission; *Technical Guidance Document in support of commission directive 93/67/EEC on risk assessment for new and existing substances. Part II*
7. Personal communication with Sten Persson; Production/logistic Manager; Stockvik Plant; Akzo Nobel Surface Chemistry.
8. Personal communication with workers at Stockvik Plant; Akzo Nobel Surface Chemistry.
9. Personal communication with Annika Star; QA manager; Stockvik Plant
10. Personal communication with Kurt Lyckeberg; Akzo Nobel Asphalt Applications; 2002
11. Personal communication with Bo Simonsson; Swedish National Road Administration; 2002
12. Zarghampour Hamid; *Handbok för återvinning av asfalt*; Vägverket publikation 2000:93
13. Personal communication with Akzo Nobel Surface Chemistry AB; 2002
14. Personal communication with Akzo Nobel Surface Chemistry AB; 2002
15. Personal communication with Eva Nabseth; Asphalt laboratory; Akzo Nobel Surface Chemistry
16. Personal communication with Matts Nordström; Special projects; Akzo Nobel Surface Chemistry; Stenungsund
17. Personal communication with Marc G.J Geurts; Research Scientist Environmental Chemistry; Chemicals Research Arnhem; 2002
18. Tests performed by Eva Nabseth at the R&D-lab for asphalt products at Akzo Nobel in Nacka, Sweden; 2002
19. Townsend T.G, Branley A; *Leaching Characteristics of Asphalt Road Waste*; University of Florida; 1998

20. Gustavsson Mats; *Icke avgasrelaterade partiklar i vägmiljön*; Report from Väg- och transportforskningsinstitutet 2001
21. Ferrante Dan; *Sorption Processes*; Civil Engineering Dept. Virginia Tech; 1996
22. Geurts, van Wijk; *Assessment of the environmental risks of Duomeen T*; General Analytical and Environmental Chemistry Department Akzo Nobel Surface Chemistry, Arnhem; 1999
23. Personal communication with Mats Norell; Akzo Nobel Surface Chemistry, Nacka.
24. Sverker Molander; Internal course in ecotoxicology for Akzo Nobel Surface chemistry; March 2002
25. US Environment protection agency homepage; *Introduction to US-EPA Ecological risk assessment*; 2002-03-21

Appendix 1

Data used in the model calculations in EUSES

Variable	Unit	Value
Chemical name		Tall oil fatty acid reaction products with polyethylenepolyamines
Product name		AA017
Cas number		68910-93-0
Tonnage substance produced in EU*	ton/year	
Tonnage substance used in EU*	ton/year	
Molecular weight*	g/mol	606
Melting point*	°C	-7
Vapor pressure*	Pa	50
Log octanol-water part.coefficient*		4.2
Water solubility*	mg/l	0.1
LC ₅₀ Daphnia (48h)*	mg/l	0.49
Biodegradability*		Inherently biodegradable
Assessment factor		10 000
Production days (2001)	days	19
Dilution in the receiving water (production)		18000

* These variables are all needed in the model calculations in EUSES.

Appendix 2

Calculations of logKow from KOWWIN

Log Kow(version 1.66 estimate): 4.21

SMILES : NCCNCCNCCNCCNCCNCCNCCN1CCN=C1(CCCCCC=CCC=CCCCCCCC)

CHEM :

MOL FOR: C34 H71 N9

MOL WT : 606.01

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	28	-CH2- [aliphatic carbon]	0.4911	13.7508
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	4	=CH- or =C< [olefinic carbon]	0.3836	1.5344
Frag	1	-NH2 [aliphatic attach]	-1.4148	-1.4148
Frag	6	-NH- [aliphatic attach]	-1.4962	-8.9772
Frag	1	-N< [aliphatic attach]	-1.8323	-1.8323
Frag	1	-N=C [aliphatic attach]	-0.0010	-0.0010
Factor	1	-C-N=C-N-C- [cyclic] structure correction	-0.6000	-0.6000
Const		Equation Constant		0.2290

Log Kow = 4.2085

Appendix 3

Another framework for environmental risk assessments -US Environmental Protection Agency (EPA)

In the United States the frameworks for the environmental/ecological risk assessment differs from those set up by the European Union. The purpose of a risk assessment in the EU is to describe and evaluate the risks of a specific individual substance on a general level. In the US the focus of the risk assessment is much more site specific. The American assessment starts with a specific goal for example, to see what the risks for one specific animal are, and then the work is to find out what can cause an effect in that specific animal. The US-EPA definition for the ecological risk assessment is “The likelihood that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors¹”. The process of ecological risk assessment is to systematically evaluate and organise data, information, assumptions and uncertainties to be able to understand relationships between stressors and ecological effects. An assessment can involve chemical, physical and biological stressors. Synergistic effects are there fore considered to a higher extent than in EU risk assessment [24]

The US-EPA guidelines for ecological risk assessments focus on stressors and effects caused by human activity. The risk assessment has three phases: problem formulation, analysis and risk characterisation and the process has two main elements: characterisation of exposure and characterisation of effects [25].

The Ecological Risk assessment process is shown in figure 6.

From the problem formulation after the available information has been investigated, assessment endpoints and conceptual models are generated. An assessment endpoint is an “expression of the actual environmental value that is to be protected” [24] Assessment endpoints are both a valued ecological unit and an attribute to that unit that is potentially at risk. The assessment endpoints can be seen as a link between the risk assessment and the risk management. The risk management is when deciding the course of action after identifying a risk. These decisions are based on many more factors than just the risk assessment results, such as social, legal, political and economical factors [25].

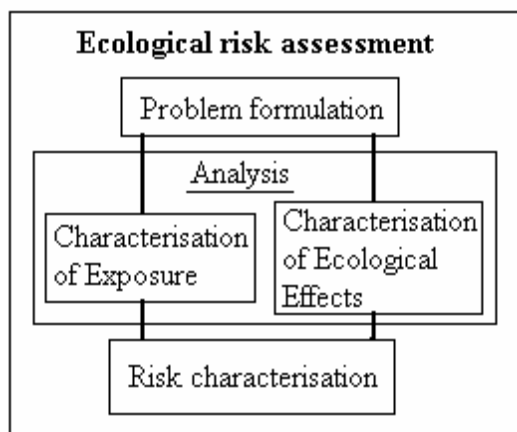


Figure 6. The US-EPA Ecological Risk Assessment process

¹ A stressor can for example be a change in PH (chemical stressor), noise (physical stressor) or a bacteria that causes a disease (biological stressor)

The process may seem straightforward and linear but the ecological risk assessment can be iterative. Something learned for example during the analysis can lead to a change in the problem formulation and so on [25].

The US guidance for ecological risk assessment is not prescriptive and there are no legal demands to perform a risk assessment [24].

Appendix 4

Warm recovery of asphalt

In an asphalt work

The most common technique in Sweden for warm recovery of asphalt is a batch-mixing work where the mixing of the recovered asphalt and the new granulate takes place in a rotary dryer. The recovered asphalt is heated by warm granulate in the rotary dryer. To this heated mass new bitumen is added. About 25 % of recovered asphalt is mixed together with new granulate and bitumen. In some works the recovered asphalt is heated in a culvert parallel to the rotary dryer and gases from this culvert are incinerated in the rotary dryer [12].

At the road

This method has three main types: repaving, remixing and remixing plus.

In the repaving the road surface is heated, cut up (depth of 20-25mm) and paved back with new asphalt on top, about 40-60 kg/m² is paved on the recovered material.

The remixing methods is similar to the repaving but here the recovered asphalt is mixed with new asphalt before it is paved back and about 30-40mm of the old surface is cut up. About 15-30 kg/m² of new asphalt is mixed into the old. In remixing plus an extra layer of new asphalt (40 kg/m²) is paved on top of the mix [12].

In all these methods, heating is done by infrared heat. During the heating of the road surface smoke is formed, so called asphalt smoke. Measurements performed on such smoke, expressed as oil mist have shown concentrations of 0.3-0.4 mg/m³.

The releases to the environment in both in situ and at asphalt works are mainly to air [12].

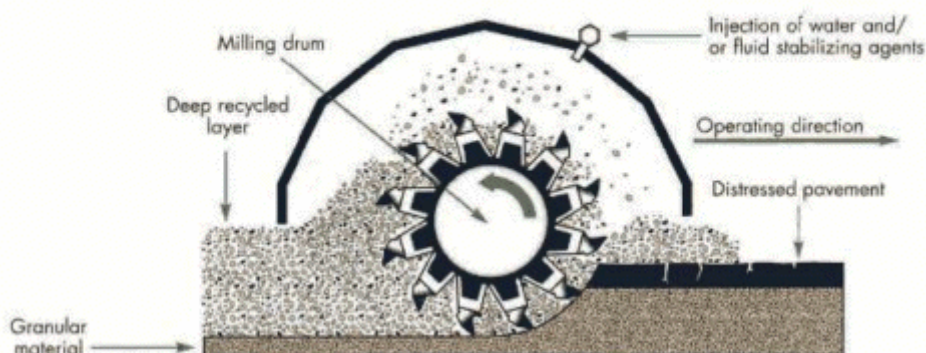


Figure 7 Cutting and milling process