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Demonstrate and Assess New Tools for Environmental Sustainability

Screening Environmental Risk Assessment applying ECETOC screening tool

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Introduction

This study examines screening Environmental Risk Assessments, ERA, for various representative data for substances produced within different units in Akzo Nobel. For more information on the substances discussed please see the confidential report.

The study was performed with the help of ECETOC[1] screening Risk Assessment tool - draft software developed based on the principles of EUSES[2]. It is a simplified tool requiring limited data. The tool can be applied for a first screening at the product portfolio in order to find out substances that require further examination. There are six different variables used in the assessment process: emission scenario, tonnage, hydrophobicity, volatility, biodegradability and ecotoxicity (See Figure 1)[3].

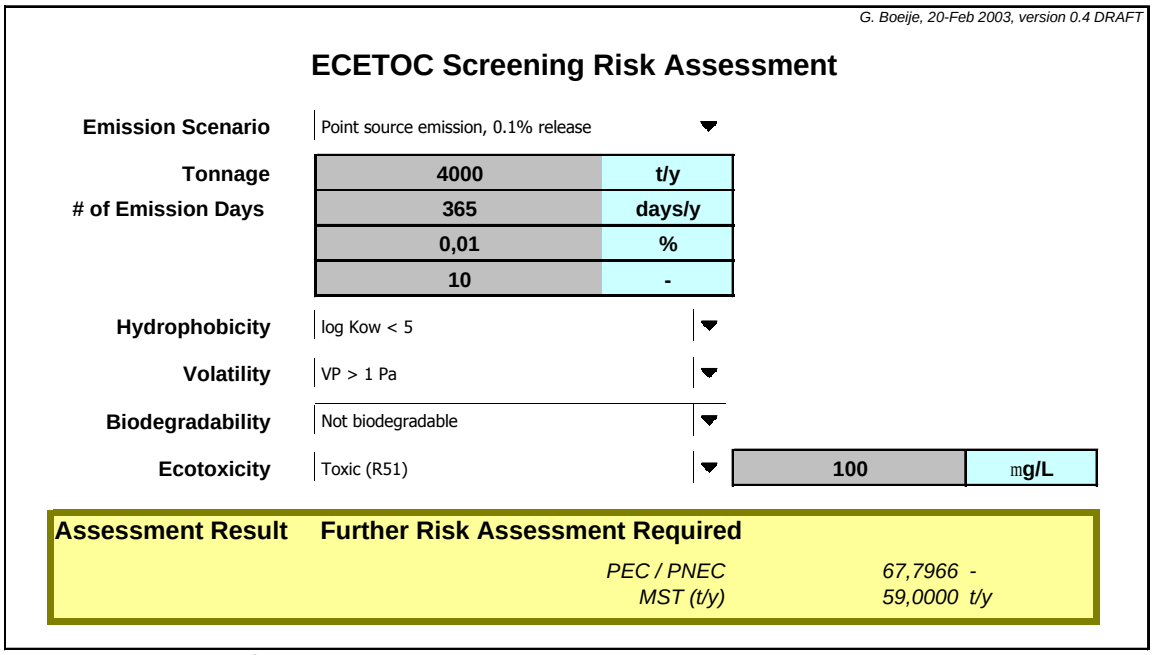


Figure 1. Screen copy from ECETOC Screening Risk Assessment tool, where
PEC = Predicted Effect Concentration
PNEC = Predicted No Effect Concentration
RCR = Risk Characterization Ratio = PEC/PNEC
MST = Tonnage/RCR

The physical data needed for using the screening tool were found in safety data sheets or estimated by experts. The sales volumes were gathered from the producers or found in different books, such as Directory of Chemical Producers, 2001.

In the report each parameter is explained, followed by the specific data for every substance. General problems, found while searching for data, are presented after the description of each parameter. The ECETOC screening tool results in RCR values which

[1] ECETOC - European Centre for Ecotoxicology and Toxicology of Chemicals
[2] EUSES, European Union System for the Evaluation of Substances, is a software program designed to be a decision-support system for the evaluation of the risks of substances to man and environment.
[3] Note: ECETOC software version 0.4 DRAFT was used.

are desired to be lower than one. The results are presented in diagrams, followed by the conclusion.

The parameters

There are six different variables used in the assessment process (see Figure 1):

1. Emission scenario
2. Tonnage
3. Hydrophobicity
4. Volatility
5. Biodegradability
6. Ecotoxicity

1. Emission scenario

One of the most important parameters in the method is the “emission scenario”. This is due to its immense influence on the RCR result. The program offers the choice between different emission scenarios mentioned below:

- “Wide dispersive use, 100% release” – this refers to activities that deliver uncontrolled exposure.
- “Point source emission, 0.1% release” – refers to the most controlled, local point source emissions, followed by 1% and 10% releases.

The release factor of 365 days per year is used in the scenarios as a default setting.

The choice of the most appropriate scenario represents the main difficulty with its application. Thus, the knowledge of all applications is needed. The solution of this problem may be, for example, to examine all the scenarios. Using all emission scenarios, it is possible to find out the maximum possible release of the substance that does not have an adverse effect on the environment.

2. Tonnage

This is a tonnage of the substance manufactured and/or imported to Europe. The tonnage is given in tons per year. The goal is to examine the total volume of the substance manufactured and/or imported to Europe. However, this type of data is limited and very difficult to obtain.

3. Hydrophobicity

Hydrophobicity shows if the substance is hydrophobic or hydrophilic. The words hydrophobic and hydrophilic literally mean 'afraid of water' and 'fond of water'. Hydrophobic materials have little or no tendency to adsorb water, while the hydrophobic possess low surface tension values and lack active groups in their surface chemistry for formation of "hydrogen-bonds" with water.

The program offers to choose between two values: log K_{ow} is more or less than 5. It should be noted that for some substances a problem of determining the value of

hydrophobicity can arise. For example, it is not possible to determine a log K_{ow} value experimentally for surfactants and inorganic substances.

4. Volatility

Volatility is the vapor pressure expressed as less than 1 Pa or more than 1 Pa.

5. Biodegradability

Biodegradability is articulated as readily biodegradable or not biodegradable. For example, inorganic substances are not readily biodegradable.

6. *Ecotoxicity*

The goal of ecotoxicity is to understand the concentration of chemicals at which organisms in the environment will be affected. This concentration should be avoided in order to protect the environment.

There are three different risk phrases given in the program to define the ecotoxicity of the substance:

R50	very toxic for aquatic organisms	(LC50 <1 mg/l)
R51	toxic for aquatic organisms	(LC50 =1-10 mg/l)
R52	harmful for aquatic organisms	(LC50 =10-100 mg/l)

The program also gives the opportunity to choose “not classified based on information.”

Representative substances’ product data

Product	Tonnage	Hydrophobicity	Volatility	Biodegradability	Ecotoxicity
Substance A	20 000	<5	>1 Pa	readily	R52
Substance B	60 000	<5	<1 Pa	NOT	R50
Substance C	3 000	<5	<1 Pa	NOT	N. C
Substance D	100	<5	<1 Pa	readily	R50
Substance E	2 000	<5	>1 Pa	readily	N.C

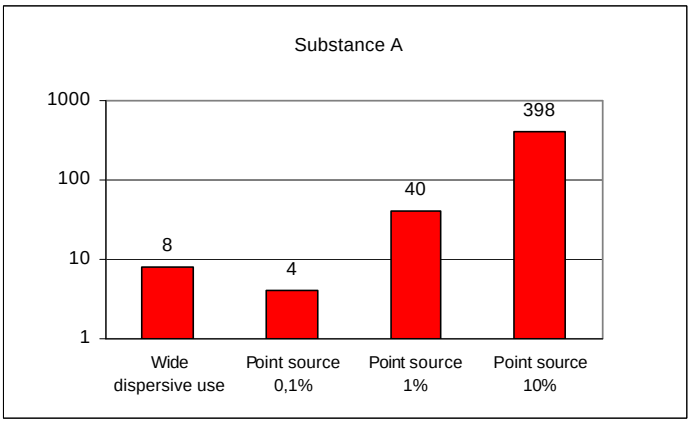
Figure 2. Data sheet. *N.C = Not classified based on information*

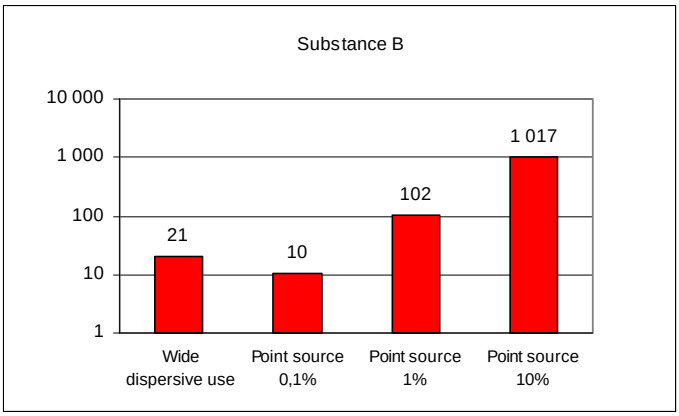
Explanation of the collected data:

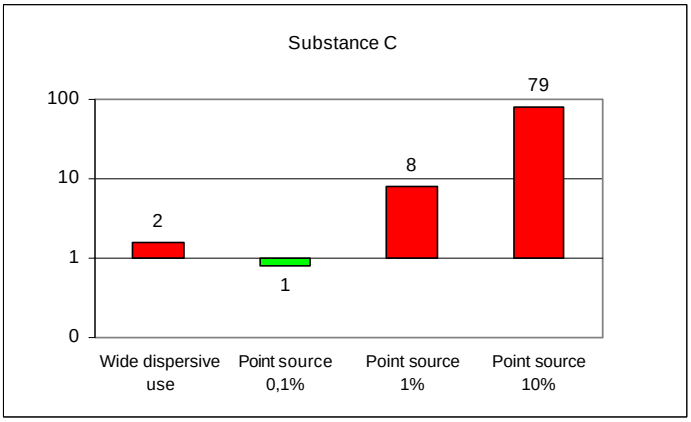
- For more exact information on the substances see the confidential report.

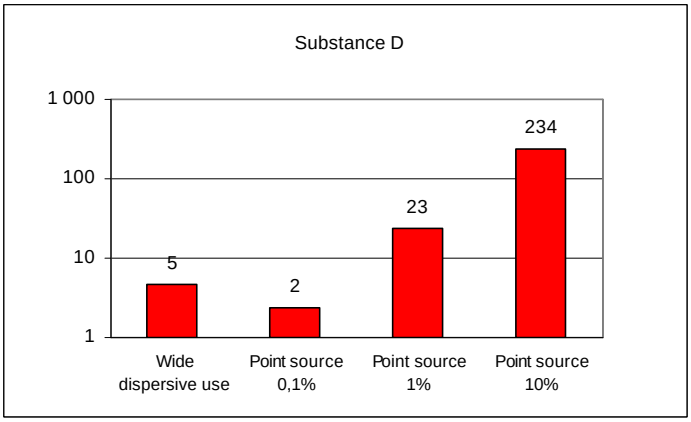
The resulted RCR, Risk Characterization Ratio, values

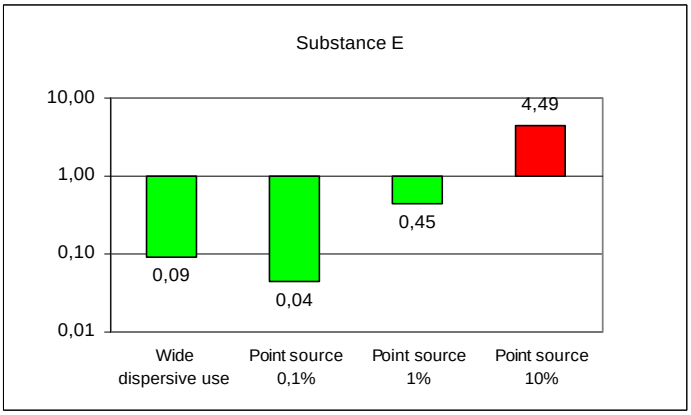
$$RCR = \frac{PEC}{PNEC}$$











Conclusion

Some of the substances have an RCR value lower than 1, which is desirable. The ones that get an RCR over one need further investigation. However, the smallest point source will have the smallest RCR value, therefore small amounts of emissions are preferable. Note that, when using the ECETOC screening tool, a wide dispersive use 100 % release, results in lower RCR values than 1% and higher point source emissions.

This study shows that the volume of the product has a huge impact on the final result. One can understand that the greater volume, the bigger will be the RCR value. It will be especially hard for the toxic and not biodegradable substances to get a low RCR value as long as they are sold in big quantities. In fact, to get a RCR value below 1, not more than about 5 tons/year of a very toxic and not biodegradable substance can be sold when having a point source 0,1 % release emission scenario. Furthermore, according to ECETOC screening tool, the largest tonnage sold of a readily biodegradable and not classified substance, can not be more than about 45 000 tons/year with a point source 0,1 % release. More details are given in the figure below.

	R50	R51	R52	NC
NOT	5	50	500	5000
readily	45	450	4500	45000

Figure 3. The chart shows the maximum sustainable tonnage per year, using a point source 0,1 % release.

It should be kept in mind that the volumes used in the study, are volumes sold by the company concerned and not the total volume in Europe. With the larger Europe volumes, the RCR values will be even higher.

It can be difficult to apply the ECETOC screening tool to surfactants and inorganic substances. This is mainly due to the complexity with the choice of log Kow and biodegradability values. It should be noted that this creates a problem for many chemical producers wishing to use the screening tool.

Moreover, ECETOC is a very simplified screening tool, which allows only rough estimations. It should be noted that the tool is still under development. Additional parameters and/or more options added to the ones already existing could result in more accurate RCR values.

More information about ECETOC screening tool can be found at the ECETOC website http://www.ecetoc.org/entry.htm. A newly published Technical Report 89 on "(Q)SARs: Evaluation of the commercially available software for human health and environmental endpoints with respect to chemical management applications" that reviews the currently-available, most preferred (Q)SAR-based predictive software can be also obtained from the ECETOC secretariat.