



## *Ministry of Transport Contaminants Database*

### *Support Manual*



MINISTRY OF TRANSPORT  
TE MANATŪ WAKA



# Ministry of Transport - Contaminants Database

Support Manual

Version 1.2

Prepared for



MINISTRY of TRANSPORT  
TE MANATŪ WAKA

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September 2000

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## Abbreviations

AET	Apparent effects threshold
ANZECC	Australian and New Zealand Environment and Conservation Council
AVS	Acid volatile sulphide
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
CAS	Chemical Abstract Service (number)
CCC	Criterion continuous concentration
CCREM	Canadian Council of Resource of Environment Ministers
CMC	Criteria maximum concentration
COPC	Contaminant of potential concern
CTV	Critical toxicity value.
EC	European Community
EIL	ecological impact level
ENEV	Environmental no effects value.
EPA	Environmental Protection Agency
EqP	Equilibrium partitioning approach
ERA	Ecological risk assessment
ER-L	Effects Range Low
ER-M	Effects Range Median
$f_{oc}$	fraction organic carbon
$g/m^3$	grams per cubic metre = parts per million
$K_{ow}$	Octanol water partition coefficient
$K_{oc}$	Octanol carbon partition coefficient
$mg/kg$	milligrams per kilogram = parts per million
$mg/m^3$	milligrams per cubic metre = parts per billion
MoT	Ministry of transport
MTBE	Methyl test-butyl ether
MW	Molecular weight
NOEC	No observed effects concentration
NOEL	No observable effects level
NPI	National Pollutant Inventory
OELD	Organisation of European Community Development
PEL	Probable Effects Level
QSAR	Quantitative structure activity relationship
SAR	Structure activity relationship
SIDS	Screening Information Data set
SLRA	Screening Level Risk Assessment
SQAL	Sediment Quality Advisory Level
SQC	Sediment Quality Criteria
TEL	Threshold Effects Levels
USEPA	United States Environmental Protection Agency
VEPA	Victoria Environmental Protection Agency (Australia)
VP	Vapour pressure

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# 1 INTRODUCTION

## 1.1 Background

This document provides background information and presents a procedure for evaluating the environmental/ecological risk associated with the presence of specific organic contaminants in the discharges and emissions from New Zealand transport sources (e.g., road and rail) to aquatic ecosystems. The document does not deal with the risk to human health or terrestrial ecosystems arising from these emissions of these contaminants.

The document supports the information presented in the associated Ministry of Transport contaminant database (TransContam-V1 and updates). It is intended that the approach outlined in this document be used in conjunction with the information compiled in the database to assist in the evaluation of new contaminants/compounds identified in emissions from road transport.

There are an extremely wide range of contaminants released as a result of the operation of motor vehicles and other transport such as rail. These include nearly all forms and classes of chemicals.

The base methodology set out in this document focuses on the assessment of single contaminants at a time. It must be recognised however that cumulative risk is important (that is, the effect of multiple contaminants acting together on an organism). It should also be noted that cumulative effects when considered should deal with the potential effects arising from exposure to all sources of contaminants not just cumulative effects for example from transport derived contaminants. As a consequence, it must be emphasised that the approach presented in this document is a screening tool.

## 1.2 Approach

This preliminary evaluation process aims to identify whether there may be a potential risk to aquatic ecosystems if a particular contaminant enters that system (i.e., is the contaminant a contaminant of potential (environmental) concern (COPC)). As will be discussed, risk and contaminant fate is a relatively complex subject particularly when it comes to quantifying risk. With new chemicals continually being introduced into our society and environment, a number of organisations have developed systems for the evaluation of existing and new chemicals. Examples of such approaches include:

1. The European Community approach to the risk assessment of new and existing substances for human and environmental effects and exposure (EU, 1993).
2. The OECD guidance for the initial assessment of screening information data for high volume chemicals (OECD 1997).
3. Australian National Pollutant Inventory (NPI) and the National Industrial Chemicals Notification and Assessment Scheme assessment process (NICNAS).

4. (<http://www.environment.gov.au/epg/npi/contextualinfo/background.html>  
<http://www.worksafe.gov.au/worksafe/08/nicnas/assesspro.html>).
5. The USEPA New Chemicals Programme (NCP) for persistent, bioaccumulative and toxic (PBT) chemicals (Office of Pollution Prevention and Toxics) (<http://www.epa.gov/opptintr/newchms/>).
6. The USEPA high production volume challenge programme which uses the OECD SIDS program approach to provide information on high volume chemical hazards in the United States .
7. The United Kingdom Department of the Environment, Transport and the Regions approach to the sustainable production and use of chemicals (<http://www.environment.detr.gov.uk/sustainable/chemicals/strategy/01.htm>).
8. The Canadian Environment Protection Act – Priority Substances Assessment Programme process for determining whether substances are toxic (Environment Canada 1997).

In New Zealand, the management of Hazardous substances is carried out by the Environmental Risk Management Authority (ERMA) under the requirements of the HASNO Act. ERMA have established an interim guide (ERMA 1999) to the specifications for hazardous substance thresholds under Act. The interim guidance identifies a number of elements of ecotoxicity that include toxicity in the aquatic environment.

The approaches utilised and developed by OECD and others have been adopted as the basic methodology for this transport/vehicle contaminant screening programme.

## 1.3 Ecological Risk Assessment

### **Definition**

The process of ecological risk assessment has been defined as:

"A process that evaluates the likelihood that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors" (USEPA 1992).

### **Framework**

Frameworks for aquatic risk assessment usually involve the following four basic evaluation steps that characterise ecological risk assessment: problem formulation, exposure assessment, ecological effects assessment and risk characterisation. A summary of these evaluation components are summarised in Table 1.1 and are overviewed in Section 2. Frameworks and approaches for ecological risk assessment have been developed and presented by a range of authors and agencies. These include USEPA (1992), EC (1994), USEPA (1996), VEPA (1997a).

**Table 1.1 - Evaluation framework (adapted from USEPA 1992).**

<p><b>Problem formulation:</b></p> <p>Problem formulation includes the identification of the source and its method of release and form; identification of the receptors and exposure pathways and identification of the endpoints to be used for assessment of effects.</p>	<p><b>Exposure assessment</b></p> <p>Exposure assessment utilises chemical measurement and chemical transport and fate evaluation or models to assess the scale, duration and frequency of exposure to the contaminants of concern. This typically involves the quantification of contaminant release, transport and fate; characterisation of exposure pathways and receptors; measurement of estimation of exposure concentrations (or intake rates) and evaluation of the quality of the data available for the exposure assessment.</p>
<p><b>Ecological effects assessment</b></p> <p>The assessment determines the relationship between the levels of exposure and effects. It can involve literature assessment and toxicity tests that identify the relationship between concentration and effects on the receptor organism.</p>	<p><b>Risk characterisation</b></p> <p>The risk characterisation links the exposure information with the effects information to provide an estimate of the risk to the receptor.</p>

## 1.4 Tiered and Compartmental Approach

Ecological risk assessments are often conducted in tiers and/or in parts. In such an approach, the simplest evaluation process is usually carried out first in a hierarchical approach. The assessment process is also often broken up into compartments such as the assessment of pathways, mode of exposure and the nature of the effects.

### **Hierarchical Approach**

A hierarchical approach can utilise a Screening Level Risk Assessment (SLRA) as the first tier of evaluation. The SLRA utilises available data to identify contaminants which require further evaluation. In the further evaluation (second tier), modelling and further data collection occurs to assess the relationship between concentration and possible effect in greater detail.

SLRA or Level 1 risk assessment is carried out for example for the initial assessment of risk at contaminated sites (VEPA 1997a). In this case, the risk characterisation consists of a comparison of on-site soil concentration data with a soil quality Ecological Impact Level (EIL). The level of soil contaminant concentration relative to the EIL defines the risk management decision as to whether conducting a higher level of assessment is warranted. The VEPA (1997a) Level 2 assessment includes the evaluation of physical, toxicological and biological parameters that affect exposure and toxicity. The VEPA (1997a) Level 3 assessment includes a literature review of the toxicological profile of the contaminants.

A number of the components that are typically included in Level 2 and Level 3 risk assessments such as those of VEPA (1997a, 1997b) have been amalgamated to provide the basis for the aquatic contaminants SLRA used in this preliminary evaluation program for transport associated contaminants.

In summary, the purpose of this SLRA is to provide a process to identify whether a specific contaminant identified as being present in an emission from a vehicle transport source is a contaminant of potential concern (COPC). As will be discussed later, this definition does not imply that the compound is a contaminant of concern.

### **Compartmental Evaluation**

As noted above, there are three key components to the assessment of ecological risk. These are the:

1. The identification of the source or sources.
2. The identification of the pathways of exposure.
3. The identification of effects.

All three require identification before a contaminant can be identified as being of concern (i.e., it is having some effect). In the contaminant database, the known sources are identified, potential pathways are assessed indirectly (via chemical properties) and the potential effects are estimated from the contaminants' properties. In this assessment process these compartments are examined theoretically. Confirmation that a contaminant is of concern requires a further level of theoretical assessment (as noted in the previous section) or actual field data on concentration or effects.

## **2. PROBLEM FRAMEWORK**

### **2.1 Introduction**

Table 2.1 provides a summary of the key topics requiring identification and evaluation in a generic ecological risk assessment. The table illustrates the complexity of the ecological risk assessment processes. Aspects of these compartments are discussed in the various sections that follow where they are included within the vehicle contaminant SLRA framework.

### **2.2 Contaminant Source**

An evaluation of the sources of contaminants associated with road and rail transport identified a number of major source categories (with each category having a series of source sub-categories). Each of the source categories and sources have been identified by a code system which is used to allow easy reference of these sources in the database. The coding system allows categories and further sources to be added in

the future. The categories for road vehicle and rail contaminant sources are summarised in Appendix A.

**Table 2.1 - Summary of ecological risk assessment components.**

<b>Risk Components</b>	<b>Sub-Components</b>
<b>Risk Population/Target:</b>	Groups of individuals Populations Multiple species Habitats and ecosystems
<b>Stressors:</b>	Single chemical Structurally related substances Structurally unrelated substances with similar target (organ, impact) effects Mixtures (dissimilar structures or mechanisms of impact)
<b>Exposure Pathways:</b> <b>(a) Pathways</b>	Air Water Food Sediment
<b>Exposure Routes for Single Organisms</b>	Ingestion (food, water) Dermal Inhalation Non-dietary intake (e.g., sediment intake)
<b>Exposure Routes for Communities/Ecosystems</b>	Direct uptake without bioaccumulation Bioaccumulation Biomagnification
<b>Endpoints:</b> <b>Effects on Populations or Species</b>	Loss of fecundity Reduced rate of growth Acute or chronic toxicity Change in biomass
<b>(b) Effects on Community:</b>	Loss of species diversity Introduction of exotic species (e.g., as a consequence on niche opening) Loss of keystone species.
<b>(c) Effects on Ecosystem:</b>	Loss of function Loss of habitat structure Loss of functional group of organisms (e.g., grazers)
<b>Time Frames:</b>	Acute Sub-chronic Chronic effects or effects with long latency periods Intermittent

## 2.3 Contaminant Type

As noted in the introduction, there are a wide range of contaminants associated with the emissions and losses from the sources identified in Appendix A. These include metals, inorganic chemicals and organic compounds. Table 2.2 provides a summary of the contaminant classification utilised for organic compounds in this assessment process.

Metals and inorganic substances will be amongst the contaminants emitted by transport sources. One of the difficulties in assessing metals within the framework of this and any other assessment process is the variety of chemical forms that the element may be present in. For example different physical states, oxidation states, chemical compounds with varying solubilities. One of the most well known metals with distinctly different properties for its different forms is chromium (trivalent and hexavalent states). As a further example Zn, which is a common component of many vehicle components is present as Zn metal, probably as divalent Zn, Zn in complex compounds present in lubricating oils and as Zn stearate in tyres and other forms. As a consequence, elements and inorganic compounds have not been included within the assessment database. As discussed later in this document, there are a range of water quality and sediment quality benchmarks for metals and other trace elements which provide readily available environmental benchmarks to assess the significance of these contaminants in the environment.

**Table 2.2 - Contaminant Classification System for Organic Compounds**

<b>Primary Category</b>	<b>Secondary Category</b>
1. Polyaromatic hydrocarbons	Unsubstituted PAHs  Substituted PAHs
2. Chlorinated organics	
3. Surfactants	Anionic surfactants Cationic surfactants Nonionic surfactants Amphoteric surfactants
4. Other organics	Acyclic hydrocarbons Cyclic hydrocarbons (non-aromatic) Alcohols Aldehydes Aromatics Carboxylic acids Ethers Ketones Phenols Quinones Silicones Sulphur compounds Nitrogen compounds Phosphorus compounds Organometallic compounds Miscellaneous organics
Composite materials	Unclassifiable

Contaminants can also be classified into their key states and classes of organic chemicals in the first instance. It is likely that a number of contaminants will be present in several states and forms. The primary states are gas, liquid and solid. In addition to these primary states, organic compounds may be present in ionic and non-ionic state and as polar and non-polar compounds. These latter compound speciations which have a significant affect on the compounds environmental behaviour (e.g., bioavailability) have not been specifically identified within the database but are taken into account in some of the properties and factors considered in the database.

This primary understanding of the nature of contaminants is important as it determines many of the contaminant's primary environmental pathways and behaviours. An example of this contrast includes the presence of metals as solid phase particulates (deposition pathway) versus metals with relatively high vapour pressures, which will be in gaseous form under the appropriate circumstances (atmospheric pathway).

## 2.4 Receptors and Endpoints

### **Receptors**

In any risk evaluation, it is not possible to evaluate the risk of a particular contaminant to all receptors or species. As such, a limited number of species are used as indicators of possible effects. In this SLRA of transport contaminants two generic environmental systems are identified:

1. Freshwater streams.
2. Estuaries and marine habitat.

The receptors should represent or be examples of key phylla or trophic levels present in those ecosystems. These are typically primary producers (algae, phytoplankton etc.), consumers (e.g., crustacea such as Daphnia) and predators (such as fish).

The selection of organisms is related mainly to what organisms are routinely used in toxicity testing for various endpoints. These are discussed in the following section. It is considered that where toxicity and other data become available for specific species present in New Zealand, that these data should be incorporated into the risk evaluation and utilised where appropriate.

### **Endpoints**

A variety of endpoints are available for use in determining acceptable risk in environmental assessments. These endpoints can occur at the individual, community or population level. This assessment process is at the individual level. Endpoints can include both acute (i.e., survival) and chronic effects (e.g., reproductive ability, growth, behaviour and physiological changes).

Endpoints such as enzymatic responses (e.g., the induction of cytochrome P450 in fish such as trout), behavioural responses (e.g., burial response New Zealand by wedge shells and lesions in individual fish may indicate contaminant exposure and response but do not necessarily provide a direct indication of adverse effects on populations and communities).

Prediction of endpoint responses in communities from other data such as survival, growth and reproductive endpoints involves a great deal of uncertainty. As such, endpoints measured in the field are typically required. Examples of the endpoints and organisms that could be utilised in this assessment programme include those identified by OELD (1995).

- ❑ 96 hour LC<sub>50</sub> for a warmwater or coldwater fish.
- ❑ 48 hour EC<sub>50</sub> for a freshwater invertebrate.
- ❑ 48 hour EC<sub>50</sub> for a bivalve embryo.
- ❑ 96 hour EC<sub>50</sub> test using an alga.
- ❑ Chronic tests for aquatic invertebrates (e.g., EC<sub>20</sub> for daphnids).
- ❑ Chronic tests for aquatic vertebrates (e.g., EC<sub>20</sub> for fish).
- ❑ Bioconcentration tests for aquatic organisms.

Endpoints for ecotoxic effect thresholds are also discussed in relation to HSNO by Reid et al (1999).

Multiple endpoints are necessary for situations where individual contaminants partition into several compartments. The MoT database includes both acute and chronic toxicity data for contaminants and information on potential bioconcentration. This is discussed further in Section 7.

## 3 PHYSICAL AND CHEMICAL PROPERTIES

### 3.1 Introduction

Basic chemical and physical data on contaminants are important as it is those properties that determine the fate of a contaminant entering the aquatic environment. As Lyman (1985) summarised, the key questions that arise in relation to contaminant fate are:

- Where does the contaminant go? and
- How fast does it get there? and in addition the following question can be added,
- How long does it stay there?

The environmental fate has a strong influence on the nature of the exposure to aquatic organisms.

A wide range of compiled data is available on physical properties for chemicals. This is available in a range of publications or can be estimated. A range of software is available to assist in the determination of some properties. Physical properties can be determined experimentally (e.g., water solubility, Henry's Law constant) (OECD 1997). However, the use of experimental methods to assess properties is not considered to be within the scope of most ecological risk screening processes (including the Transport Contaminant database). The availability of information on properties allows the fate and transport to be assessed to the point where decisions can be made about the environmental significance of the contaminant.

The following sections identify and describe the key properties that are required to assess ecological risk in aquatic systems (and those presented in the database), describes sources of information and identifies some of the means by which the properties can be estimated.

## 3.2 Properties

Table 3.1 provides a summary of the physical and chemical property data presented in the database and used in the assessment database to evaluate aquatic ecological risk. The commentary set out below has assumed that the contaminants are present in low concentrations and that they are not present as separate phases. The CAS (Chemical Abstract Service) number is identified in the database where known. CAS numbers can be identified through a number of databases (e.g., Chemfinder at <http://www.chemfinder.cm/>). There is a range of other properties (e.g., the acid dissociation constant) that provide useful information on the fate of organic compounds. These are not included in the current database but can be added in due course by users.

**Table 3.1 - Summary of physical/chemical properties used in the database.**

<b>Property</b>	<b>Unit</b>	<b>Abbreviation</b>
Phase/State	-	S, L or G
Molecular Weight	g/mol	MW
Melting Point	°C	T <sub>m</sub>
Boiling Point	°C	BP
Density/Specific gravity	g/m <sup>3</sup>	SG
Vapour Pressure	mm Hg	VP
Solubility	g/m <sup>3</sup>	S
Henry's Law Constant Dimensionless H'	atm m <sup>3</sup> /mol	H'
Organic Carbon partition coefficient	L[water]/L(Organic carbon]	K <sub>OC</sub>
Octanol-Water partition coefficient	L[water]/L(Octanol]	K <sub>OW</sub>

### **Bulk state**

The form of the contaminant is important in the determination of fate and effect. In the database, the form or state is recorded as solid (S) (e.g., particulate, debris from tyre and brake pad wear; particulates in exhaust emissions), liquid (L) (e.g., in oil, brake-fluid components) or gas (G) (e.g., in evaporation or exhaust components).

### **Molecular Weight (MW)**

The MW can be obtained from a variety of references or calculated from the contaminants' structural formula. The calculation can be carried out manually or using a molecular weight calculator (there are numerous available through the internet).

### **Density/Specific Gravity (SG)**

The density or SG of contaminants is expressed as g/cm<sup>3</sup>.

### **Water Solubility (S)**

Aqueous solubility is an important property that determines a chemical's toxicity, sorption characteristic, bioaccumulation and phase equilibria. All compounds are soluble to some extent. The S is the upper limit of the dissolved concentration in water at a specified temperature (concentration when the solute is in equilibrium with the pure (undissolved) compound). It should be noted that the total concentration in water can exceed this value under certain circumstances. These include adsorption to particulate matter and the presence of solvents which, increase the apparent solubility in water.

Very low solubilities have been reported for chemicals such as benzo(g,h,i)perylene (0.26 mg/m<sup>3</sup>). Some compounds such as ethyl-alcohol are infinitely soluble. Consequently the solubility of organic compounds ranges over several orders of magnitude. Measured S values are presented in a number of references and can be obtained from databases. Lyman et al. (1982) and Lyman (1985) discuss methods to estimate S where no data can be found. S can be estimated from structure and is generally inversely related to the octanol water partition coefficient ( $k_{ow}$ ).

### **Melting Point (Tm)**

Tm is a measured parameter available for most chemicals in the literature data as presented as °C.

### **Vapour Pressure (VP)**

VP is the pressure exerted by a chemical vapour in equilibrium with its liquid or solid phase. The VP is an important factor that determines the rate at which a chemical volatilises from sediment or water. It is also used to estimate the Henry's Law Constant (H') for low solubility chemicals. The higher the VP is, the higher the probability that the chemical will exist in the gas phase. The VP is a function of temperature and molecular weight and can be estimated (Lyman et al. 1982, Lyman 1985).

### **Henry's Law Constant (H')**

The Henry's Law constant describes the partitioning of a contaminant between air and water at a defined temperature. H' is often expressed as the partial pressure of the chemical in the gas phase divided by the concentration in the liquid phase. For

chemicals with low solubilities in water,  $H'$  can be estimated from the VP of the chemical divided by the solubility limit in water. The higher  $H'$ , the more likely the chemical is to exist in the gas phase than in water. Methods to estimate  $H'$  can be found in Lyman et al. (1982) and Lyman (1985).

The temperature that  $H'$  is reported as should be appropriate to the environment. For the purpose of this assessment process as temperature varies throughout New Zealand, a default temperature of 25 °C has been used (wherever possible) as this is at the upper limits of expected water temperatures in all areas of New Zealand.

$H'$  can also be estimated as the ratio of measured vapour pressure (VP) to water solubility (S) as  $H = VP/S$ .

### **Adsorption Coefficient ( $k_{oc}$ )**

The tendency of a contaminant to be adsorbed is expressed as the  $k_{oc}$ . The  $k_{oc}$  is the ratio of the amount of contaminant adsorbed per unit weight of organic carbon in the soil/sediment to the concentration in water at equilibrium.  $k_{oc}$  values range over 6 orders of magnitude.  $k_{oc}$  is an important factor in the assessment of fate.  $k$  can be calculated from a measured adsorption isotherm and from  $k$  the  $k_{oc}$  ( $= k/\%$  organic carbon, typically standardised to 1%).

### **Octanol/Water Partition coefficient ( $k_{ow}$ )**

The  $k_{ow}$  is an important property as it 'determines' the partitioning/movement of the chemical between water and fat (lipid). Octanol has a carbon to oxygen ratio very similar to lipid and is only sparingly soluble in water (about 600 g/m<sup>3</sup>). As a consequence those chemicals with a high  $k_{ow}$ s tend to bioaccumulate in organisms with high lipid contents.

The organic carbon/water partition coefficient ( $k_{oc}$ ) can be calculated from the  $k_{ow}$  if required. Lyman (1985) describes methods to calculate  $k_{oc}$  and  $k_{sw}$  (the soil/water partition coefficient). For non-ionic organic compounds,  $K_{oc}$  is empirically estimated to be 0.48 times  $K_{ow}$ . This is not included in the database.

## 3.3 Sources of data on chemical properties

Data on the measured (experimental) physical and chemical properties of chemical species can be obtained from a variety of sources including published literature. A number of specific books have been published from which data can be extracted (e.g., CRC Handbook of Chemistry, Merck Index, Verschueren (1983). In this screening assessment the Merck Index (1996) was used where required to obtain data. Information on some chemical species can be obtained by carrying out literature searches where experimental data are specifically required.

There are methods for obtaining experimental data for the properties identified in this screening process (e.g., refer OECD guidance methods for estimation of physical and

chemical properties of new chemicals). These properties have been measured as part of new chemical evaluations and also as part of chemical and environmental studies.

There are a variety of databases/software that have compiled measured data that can be used to access physical properties data for identified compounds. These include:

- ❑ Toxnet (National Library of Medicine) <http://toxnet.nlm.nih.gov/servelets/simple-search> provides internet access to a wide range of information on chemical species through a number of search engines/databases. The Hazardous Substances Database (HSDB) is the main source of environmental data. The output includes synonyms and a wide range of physical and chemical properties plus some environmental fate information.
- ❑ Chemfinder (<http://www.chemfinder.com/>) is a well established search system with extensive links to information on the chemical and physical properties of chemicals.
- ❑ Chemfate ([http://es\\_plaza.syrres.com/efdb/Chemfate.htm](http://es_plaza.syrres.com/efdb/Chemfate.htm)), is a search database that contains information on 25 categories of environmental fate and physical properties on commercially important chemical compounds. Developed and managed by Syracuse Research Corporation.
- ❑ Datalog ([http://es\\_plaza.syrres.com/efdb/DATALOG.htm](http://es_plaza.syrres.com/efdb/DATALOG.htm)) is a bibliographic information base containing 18 different types of environmental fate data. Developed and managed by Syracuse Research Corporation.
- ❑ Biolog ([http://es\\_plaza.syrres.com//BIOLOG.htm](http://es_plaza.syrres.com//BIOLOG.htm)) is a source of information on microbial degradation and toxicity information. Developed and managed by Syracuse Research Corporation.

The USEPA National Risk Management Laboratory has developed a database on the effectiveness of treatment technologies for removal/destruction of chemicals in a range of media. The treatability database (TDB) is accessible at <http://www.epa.gov/tdbnrmrl/> and provides information on a number of physical and chemical properties of a set number of chemical species (it does not provide data for compounds not in its database).

There are a number of specific sources of particular properties. For example, data on H' can be obtained from R Sanders listing at <http://www.mpch-mainz.mpg.de/~sanders/res/henry.html>.

In addition to web-based search systems, there are a number of commercially available packages from which data can be extracted. These include:

- ❑ Chemrank (School of Resource & Environmental Management, Simon Fraser University, BC). A chemical risk ranking programme that contains data on a variety of chemical species.
- ❑ ToxChem (Enviromega Inc, Ontario), is a wastewater contaminant fate (within treatment plant) expert system that contains properties for a range of chemical species within the programme.

Where these or other sources were used to provide information for the database, the reference is provided in the database.

### 3.4 Estimating Properties

Data are not always available on physical properties for some compounds. As noted earlier experimental methods are not appropriate for estimating physical properties as part of contaminant SLRA. As a consequence, computer based methods and models are the quickest method to estimate key properties.

The relationship between structure and property is used as the base for estimating the properties of chemicals for which data is required. The models are referred to as Quantitative Structure Activity Relationships or QSARs. The QSAR approach is based on the properties of functional groups and as such requires structural information about the compound structure and individual functional groups in the chemical. There are a variety of QSAR models that utilise different theoretical approaches (for example group or atom/fragment contribution methods). The following programmes can be used to estimate individual factors for specific chemicals:

#### **MP, BP and VP**

Melting point, boiling point and vapour pressure can be estimated using MPBPVP developed by Syracuse Research Corporation (<http://www.syrres.com>). The programme uses CAS number or chemical structure in SMILES notation.

#### **K<sub>ow</sub>**

K<sub>ow</sub> (Octanol/water partition coefficient) can be estimated using computer programmes such as ClogP (Biobyte Corporation), EPIWIN, KOWWIN (Syracuse Research Corporation). KOWIN calculates the octanol/water partition coefficient using the atom/fragment contribution method (Meylan & Howard 1995).

#### **S**

Water solubility can be calculated using WSKOW (Syracuse Research Corporation). The methodology is described in Meylan et al. (1996).

#### **k<sub>oc</sub>**

The soil organic carbon partition coefficient can be calculated using the programme PCKOCWIN (Syracuse Research Corporation). The method is reported in Meylan et al. (1992).

#### **H'**

Henrys Law constant can be estimated using the programme HENRYWIN (Syracuse Research Corporation). HENRYWIN uses an updated version of both the group contribution and bond contribution methods of Hine & Mookerjee (1975, after Meylan & Howard 1991).

## Multiple Properties

A range of physical and thermodynamic properties can be obtained for a wide range of organic compounds in the programme Physprop (G & P Engineering Software). Chemdat 8 (or 9) is a USEPA DOS based program that uses the Uniquac Functional group Activity Coefficient (UNIFAC) model to estimate a wide range of properties for a range of compounds in its database.

ASTER (Assessment Tools for the Evaluation of Risk) is an ecotoxicological support system developed by USEPA for environmental risk assessment. ASTER is an integration of the AQUIRE toxic effects database (refer above) and the QSAR system, a structure activity based expert system. ASTER is designed to produce high quality data for individual chemicals. ASTER uses QSAR when data in its database is absent. ASTER is a VAX based system. ASTER provides and calculates data for a range of properties including Tm, BP, VP, Water solubility, pka, K<sub>oc</sub>, Henrys constant, hydrolysis half life, fugacity.

Where a specific programme has been used to estimate a property for a compound in the database, the programme/reference is provided. For example all BCF values used in the database were calculated using BCFWIN. The key properties of the chemical compounds within the database are presented in the first main screen of the Transport Contaminant database as shown below.

The screenshot shows the 'Contaminants' database interface. At the top, there are buttons for 'Find A Contaminant' and 'Enter A New Contaminant'. Below these is a search bar with 'mercaptobenzothiazole' entered. The main area displays various properties for this compound:

Synonyms:	2-benzothiazolethiol; 2[3H]-benzothiozolethione;	
CAS Number:	00149-30-4	
Category Code:	Road: 4.1; 8.1	
	Rail: 4.1	
Chemical Class:	Sulphur Compound	
Physical State:	liquid	
Molecular Weight:	167.2432	g/mol
Melting Point:	179	degrees C
Boiling Point:	311	degrees C
Vapour Pressure:	8.19E-05	mm of Hg
Specific Gravity:	1.42	g/cm3
Solubility in Water:	98.66	g/m3
Henry's Constant:	0.00000141	atm-m3/mol
Kow Octanol/Water Partition Coefficient:	2.42	
Koc Water/Carbon Partition Coefficient:	2.94	

A 'References' button is located on the right side of the property list.

## 4 TOXICITY DATA

### 4.1 Exposure Assessment

The two key endpoints in aquatic exposure assessment are chronic and acute toxicity.

- Acute exposure is a short-term exposure, usually lasting less than 96 hours.

- Chronic exposure is longer and can be a relatively significant proportion of an organisms life-span.

Both exposure categories are relevant, as the chronic toxicity will typically occur over a larger area from the contaminant source compared to the acute toxicity.

## 4.2 Water Exposure

### 4.2.1 Introduction

Toxicity of some contaminants (e.g., certain metals) is dependent upon water chemistry. Such factors include pH and hardness. Hardness has been accounted for in the development of criteria for those metals whose toxicity is known to be dependent upon hardness (USEPA 1996).

Changes to toxicity along exposure pathways should where possible be taken into account. If not, the overall risk assessment may tend to be conservative with respect to those contaminants. In this SLRA, other factors such as degradation are considered in relation to persistence but are not considered directly in the toxicity assessment.

### 4.2.2 Endpoints

One of the difficulties in screening procedures is identifying what range of organisms and what level of protection should the screening or benchmark concentrations protect in aquatic ecosystems. As noted by Sample et al. (1998), there are a variety of benchmarks available to use in the assessment of potential effects. Their use depends upon whether they are conservative and on the quality of the data that they have been derived from.

In relation to those endpoints, which are related to aquatic toxicity, it is useful to determine a single endpoint which represents the critical toxicity value. Suter & Tsao (1996) present toxicological benchmarks for a variety of contaminants and discuss their derivation. The endpoint is an estimate of low toxic effect and are typically endpoints such as LC<sub>25</sub> or IC<sub>25</sub> values or NOEL (the NOEL [no observed effect level] is the highest concentration of a contaminant not to cause a statistically significant effect compared to a control) or LOEL (the LOEL [lowest observed effects level] is the lowest concentration in a toxicity test that results in a statistically significant effect when compared to the controls) values.

Values such as those noted above can be used to determine a critical toxicity value (CTV). This value is not a no-effects concentration value. This approach is used by Environment Canada (Environment Canada 1997) in its approach to screen Priority Substances. The CTV can be used as a first tier to assess whether a compound is likely to be a concern in the environment (e.g., CTV/Environment Concentration is >1). In the database, the CTV is identified as the lowest value within the database – presumably the most sensitive species assessed.

The CTV can be used to identify an ENEV (Environmental No Effects Value). This value can be derived using application factors. Table 2.3 summarises the application

factors identified by Environment Canada (1997). In this assessment, the database identifies the CTV as the lowest chronic toxicity data-point within the data set presented.

This value is then divided by a factor of 10 if the CTV is based upon a chronic toxicity value derived from a set of data encompassing a range of phylla (refer Table 4.1). In some cases a factor of 100 is utilised if the CTV is based upon acute toxicity. The ENEV can then be compared to environmental data to confirm whether the contaminant is a contaminant of concern. This is discussed further later in this document.

**Table 4.1 - Maximum application factors recommended by Environment Canada (1997).**

<b>Level of Information</b>	<b>Maximum recommended application factor</b>
Threshold of sublethal toxicity data such as IC <sub>25</sub> comes from a base data set (e.g., fish, daphnid and algal species)	10
Lowest acute LC <sub>50</sub> or EC <sub>50</sub> from a database set (e.g., fish, daphnid and algal species)	100
Lowest acute LC <sub>50</sub> or EC <sub>50</sub> comes from a data set of one or two species	1000

In this contaminant database, the use of endpoints does not identify whether a particular contaminant is a COPC. As will be discussed later, final assessment of concern requires environmental information of some kind (e.g., discharge or receiving environment concentration data).

#### **4.2.3 Water Quality Guidelines**

A range of guidelines have been developed around the world to protect aquatic biota from exposure to toxicants. In New Zealand guidelines and criteria developed by USEPA, CCREM and ANZECC have received the most use. The number of toxic substances for which guidelines and criteria have been developed is restricted. Guidelines are available for the key metals, a range of semi-volatile organochlorine compounds, PAHs and selected VOCs. Where guidelines or criteria are available, these are reported in the data-base. Identification of a criteria or guideline in the data-base indicates that the contaminant has already been identified as a potential contaminant of concern at the concentration specified (and under the conditions specified by the particular guideline or criteria) (also refer section 8).

#### **United States Environment Protection Agency**

The United States Environment Protection Agency (USEPA) develops water quality criteria as a requirement of Section 304(a)1 of the Clean Water Act. The Clean Water Act recognises a series of priority toxic pollutants. The criteria which were derived by the USEPA can be adopted by the States in their formal water quality standards. The USEPA approach is one of endeavouring to protect 95% of all freshwater and marine organisms in the United States. The process of developing the criteria is flexible in that

it can be adjusted to provide differing levels of protection depending on the nature of the ecosystem involved. The USEPA criteria provide protection against acute (short term) and chronic (long term) toxicity. These are referred to as the Criterion Maximum Concentration (CMC) and the Criterion Continuous Concentration (CCC) respectively.

The area in which there has been the most significant change within the USEPA guidelines has been their interpretation in relation to environmental toxics data for metals. The criteria were originally developed with field data being collected as total recoverable metals. This was then amended to require measurements to be in the form of acid soluble. Recently following debate, this was amended again to require the analytical data used to compare against the criteria to be in dissolved form. This change occurred as the previous forms of measurement were considered to be over-protective. Procedures are available to adjust criteria to account for dissolved measurement and comparison with the criteria.

### **Canada**

The Canadian water quality guidelines are a set of values that have been developed to protect all forms of aquatic life and all components of those organisms life cycles. As such they differ from the USEPA criteria in that they are intended to protect all organisms. The guidelines are therefore no-effect concentrations and protect against chronic effects, fish bio-accumulation and fish tainting. Where insufficient chronic toxicity data was available, an application factor was utilised to develop the chronic value from acute toxicity data. CCREM (1991) were not intended to be overall national values but were intended to be utilised to develop site specific guidelines. CCREM have recently updated their water quality guidelines (CCREM 1999). The key difference to the USEPA approach is the use of a not to be exceeded maximum value rather than the two tiered (acute and chronic) approach. As such, the guidelines are lower than USEPA criteria.

### **ANZECC**

The Australian and New Zealand Conservation Council (ANZECC) developed a series of water guidelines for the protection of a wide range of ecosystem and use values (ANZECC 1992). Guidelines for those parameters that are toxic or able to be bioaccumulated were developed using the methods of CCREM (1991). As such, the guidelines were developed to protect all organisms. As with the Canadian approach, application factors were utilised where there was insufficient chronic toxicity data. At the time of the completion of this document, ANZECC have released the ANZECC (2000) water quality guidelines. The ANZECC (2000) criteria can be added to the database.

For completeness, the water quality criteria developed by the USEPA and the CCREM (1999) are included within the database where they are available for identified contaminants.

## 4.3 Sediment Exposure

### 4.3.1 Endpoints

The presence or build-up of contaminants in sediment has the potential to result in:

1. Acute toxicity.
2. Chronic toxicity.
3. Chronic non-toxic effects.
4. Bioaccumulation.

The exposure relating to one of these end-points may occur as a result of exposure to one of three key compartments in the sediment contaminant reservoir. These are:

1. Contaminant adsorbed or absorbed to particulate material.
2. Contaminant in the sediment pore water.

A simplified overview of the link between the end points and the sources of sediment associated contaminants is presented in Table 4.2.

**Table 4.2 - Summary of end points.**

<b>Source</b>	<b>End Point</b>	<b>Key Path/Consumer</b>
Pore Water	Toxicity	Benthic invertebrates Benthic sediment grazers
Sediment	Bioaccumulation	Benthic sediment grazers Predators of benthic grazers

Whole concentration of contaminant in sediment can be used to assess potential toxicity or the sediment pore water concentration can be used to assess potential toxicity. Sediment pore water concentration of a contaminant is considered to be a more direct measure of sediment toxicity to benthic organisms. Estimates of exposure to elevated concentrations of contaminants in sediment pore waters are typically estimated from whole sediment concentrations. There are a variety of ways to theoretically estimate sediment pore water concentrations. Such estimates have been used to estimate sediment quality.

### 4.3.2 Sediment Quality Standards

Sediment quality guidelines have been developed to assist in the interpretation of sediment quality data. The key reason for the development of sediment quality guidelines has been the identification of potential adverse impacts of sediment quality on benthic invertebrate ecological health. Adverse effects may include toxicity and bioaccumulation. Sediment screening guidelines have been developed using a number of different methods. Irrespective of the method used, the guidelines have been developed to identify sediment contaminant concentrations at which adverse effects could occur in benthic invertebrate communities. Suter et al. (1998) provides comment on the nature of sediment quality benchmarks.

Examples of sediment screening guidelines include:

1. Apparent effects thresholds (AETs) for a selection of organic compounds and metals developed by Barrick et al. (1988). The AET approach utilises any field or laboratory effects data and compares it to sediment quality data. The guidelines were developed for Puget Sound in Washington State.
2. Effects Range Low (ER-L) and effects range median (ER-M) developed by Long & Morgan (1990) and Long et al. (1995) for a range of metals and organic compounds. The effects range values were derived by utilising data from field environmental effects data, laboratory studies, and also equilibrium partitioning data. The ER-L is the 10<sup>th</sup> percentile and the ER-M the 50<sup>th</sup> percentile of the data examined by those authors. Effects range guidelines are available for a number of contaminants including the key trace elements and PAHs identified as derived from road transport. Extensive field verification of the accuracy of prediction has been carried out (Long et al. 1995 in USEPA 1997). Toxicity testing of a large number of samples demonstrated that the toxicity increases as the number of chemicals exceeded the ER-L or ER-M.
3. Draft sediment quality criteria (SQC) developed by the USEPA using the equilibrium partitioning approach. A total of five draft SQC have been developed. These are for acenaphthene, fluoranthene, phenanthrene and two organochlorine compounds (aldrin and dieldrin). Further information can be found in Di Toro et al. 1991, 1992).
4. Sediment quality advisory levels (SQALs) for a number of nonionic organic compounds developed by the USEPA (USEPA 1992, 1993) using the equilibrium partitioning approach. For contaminants other than the five for which the EPA developed SQC values, an advisory level was calculated for use as a screening tool.
5. Threshold effects levels (TELs) and Probable effects levels (PELs) developed by the Florida Department of Environmental Protection (FDEP 1994). These guidelines were developed for the Florida coastal environment using a similar approach to that used by Long et al. (1990). FDEP (1994) should be referred to for further details. The effectiveness of the two guidelines at predicting toxicity was assessed by Long et al. (in USEPA 1997).
6. CCREM (1999) have identified a range of guideline values similar to those of Long et al. (1995). The guideline concentrations cover both freshwater and marine sediments.

For completeness, the sediment quality guidelines developed by Long et al. (1995) and CCREM (1999) are provided within the Transport Contaminant database. In contrast to the water quality guidelines, there is less certainty with regard to the probability of effects at concentrations above the sediment quality guidance value. The identification of a guidance value generally indicates that at sufficient concentration, the contaminant is a contaminant of concern.

## 4.4 Toxicity Data

Toxicity data is available from a variety of sources. Data for specific compounds and elements can be sourced from the literature or from compilations of toxicity data (e.g., gathered for the formulation of water quality standards and guidelines). Such compilations may contain a large amount of toxicity data and it may be necessary to screen the data for that for the identified end-points. Toxicity data can also be theoretically derived. As with the derivation of data for physical properties, QSARS may be used to predict the effects of chemical substances. QSARs can be used to make initial estimates of toxicity and to determine whether further assessment is done. Reid et al. (1999) discuss the use of QSARS for determining aquatic toxicity.

In this preliminary contaminant evaluation process, toxicity data was derived from two key sources:

1. ECOSAR (Ecological Structure Activity Relationships) is a software program used to estimate the toxicity of chemicals discharged into water. The programme predicts the toxicity to organisms such as fish, invertebrates and algae using SARs. Both acute and chronic toxicity can be estimated. SARs express the correlations between a compounds physico-chemical property and its aquatic toxicity. SARs measured for one compound can be used to predict the toxicity of similar compounds belonging to the same chemical class. ECOSAR requires data for MW and  $K_{ow}$  and structure. Structure is defined using SMILES notation (Simplified Molecular Input Line Entry System).
2. ASTER (refer above), provides toxicity data for a number of species (e.g., water flea and rainbow trout) for a number of acute and chronic end-points.

Another QSAR programme TOPKAT (Heath Designs Inc.) can provide estimated toxicity data for Daphnia ( $EC_{50}$ ) and for fathead minnow ( $LC_{50}$ ).

In addition, to these programmes, searching the USEPA database ECOTOX (Pugilisi et al. 1996) can also provides data. ECOTOX is a significant expert system established by the USEPA that integrates information in three key databases (AQUIRE, PHYTOTOX and TERRETOX). The system allows the extraction from the USEPA databases of specific information on single chemical species to be extracted easily. Until recently this system was not directly open to use through the internet. AQUIRE (Aquatic Information Retrieval Database) extracts data from a wide variety of literature sources and includes acute and chronic data, bioaccumulation and sublethal effects data for both marine and freshwater aquatic species. PHYTOTOX is a database (compiled from the literature) that provides data on the effects of organic chemicals on plants (compiled by Department of Botany and Microbiology at the University of Oklahoma on behalf of USEPA).

The former two sources of information provide calculated toxicity data. In the context of the providing a screening of the compounds, such approaches provide sufficiently robust information to aid in the identification of contaminants of concern. Within the Transport Contaminant database, the source of the actual/estimated toxicity data is identified in pull down references.

**Contaminants** Find A Contaminant Enter A New Contaminant Quit

Select Compound: mercaptobenzothiazole

**Acute toxicity**

Species	Test Time	Effect	Endpoint	Concentration mg/L	Reference
Fish	4	MOR	LC50	7.254	1
Daphnid	2	MOR	LC50	4.005	1
Green Algae	4	MOR	LC50	14.396	1
Daphnid	2	MOR	LC50	9.307	2
Bluegill	4	MOR	LC50	13.236	2
Fathead minnow	4	MOR	LC50	16.661	2

Record: 1 of 8

**Chronic toxicity**

Species	Test Time	Effect	Endpoint	Concentration mg/L	Reference
Fish	30	GRO	EC50	1.084	1
Fish	90	GRO	CHV	0.082	1
Daphnid	21	GRO	EC50	0.784	1
Green Algae	96	GRO	CHV	2.367	1
Fathead minnow	32	GRO	MATC	2.762	2

Record: 1 of 5

CTV 0.082  
ENEV 0.0082

Toxicity References

## 5 FATE

Assessment of fate requires information in relation to a number of different processes that influence the route that the chemical species takes within the environment when released. Typically, the key factors/processes that need to be considered include:

1. Dilution.
2. Degradation.
3. Adsorption.
4. Volatilisation.

### Dilution

Dilution is the primary process that determines the overall effect of a specific chemical within a given environmental compartment. With information on fate (determined by factors such as Henry's law constant,  $K_{oc}$  etc.), the proportional concentrations within a given compartment can be calculated. Such principles are utilised within environmental fate models to assess distribution of chemicals released/discharged to the environment.

### Degradation

Degradation of organic and inorganic compounds occurs via both biotic and abiotic processes. Biotic processes include microbial degradation and abiotic processes include photolysis and hydrolysis. OECD (1998) defines degradability in terms of

overall degradation requiring specific degradation tests to be conducted. Specific aspects of degradation can be assessed. For example:

- BIODEG/BioWin (Syracuse Research Corporation), which estimates the probability that a chemical under aerobic conditions and micro-organisms will biodegrade.
- Hydro (Syracuse Research Corporation), which estimates hydrolysis rate constants and half lives for specific organic compound classes (e.g., esters).

Aster provides output for certain aspects of degradation using programmes such as these (refer section 3.3).

### **Adsorption**

Adsorption can be assessed through the relative value of the  $k_{oc}$  value (refer section 3.2).

### **Volatilisation**

Volatilisation is a key property that determines the fate of organic compounds. Two measures are utilised in the database to assess the degree of volatilisation. These are the compound VP and Henry's Law constant (refer section 3.2).

### **Fugacity**

The partitioning of specific chemicals released to the environment can be assessed using fugacity models. The development of a partitioning model based upon the concept of fugacity was carried out by Mackay (1982) and Mackay et al. (1983). Chemical equilibrium or partitioning between two phases is expressed as the "escaping tendency or pressure" that the chemical exerts in any given phase. In equilibrium, the fugacity in each compartment is the same. Fugacity is expressed as a partial pressure and the partition coefficients are then expressed as the ratio of the compartment fugacities.

Fugacity models can range from simple to very complex depending upon the needs of the model and the factors that are taken into account (MacKay et al. 1983). In the simplest model, the fugacities are calculated for each of the compartments and of the model ecosystem; the distribution of the contaminant is then calculated within the compartments. In this assessment, a Level 1 fugacity model (also called a Mackay Level 1 model) with six compartments is used to calculate the environmental distribution of a chemical at equilibrium and steady-state. The six compartments are air, soil, water, sediment, suspended solids and fish.

The proportional distribution of the chemical within the water compartment provides information in relation to the overall fate within the aquatic system. The proportion within water also provides additional information on risk to aquatic organisms via toxicity. The key properties utilised to assess fugacity in water compartment include solubility, vapour pressure and Henry's Law constant (refer Section 4) and for biota (bioconcentration factor) amongst other things.

A screen shot from the Transport Contaminant database is provided below showing the fugacity partitioning data output. The output provided in this area of the database is not used in the specific assessment of individual contaminant risk and concern. The information is provided to provide a more complete picture of the fate of the particular compound. Fugacity/partitioning data is not able to be provided if key data (e.g., VP) is missing from the properties database.

## 6 BIOACCUMULATION

Bioaccumulation (the process whereby a chemical is taken up from an environmental media into an organism) is a key factor affecting the overall assessment of risk associated with organic compounds. Bioaccumulation or a chemical's ability to bioaccumulate has the potential to result in adverse effects on an organism or can result in the transfer of contaminants up food chains as a consequence of consumption of the organism by a predator (biomagnification) or consumption by humans.

Bioaccumulation is a relatively complex phenomenon affected by a variety of factors (refer Carey et al. 1998). Key factors are polarity, hydrophobicity and metabolic rate. Bioaccumulation from water is important as large gradients exist between water and biota for hydrophobic organic compounds. Although bioaccumulation can differ between organisms with differing feeding habits and between freshwater and marine fish (due to differences in their physico-chemical environment), bioaccumulation data can be obtained experimentally and from field data. Even with all of the environmental and biological variables affecting bioaccumulation including both environmental and biological transformation of the contaminant, approximations of bioaccumulation potential are valuable in assessing ecological risk associated with uptake.

The screenshot shows the 'Contaminants' database interface. At the top, there are buttons for 'Find A Contaminant', 'Enter A New Contaminant', and 'Quit'. Below these is a search bar with 'mercaptobenzothiazole' entered. The main content area is divided into three columns: 'Properties', 'Toxicity', and 'Persistence and Bioaccumulation'. The 'Persistence and Bioaccumulation' column contains the following data:

Category	Value	Unit
Hydrolysis Half Life	Hydrolysis unlikely	half life days
BOD Half Life	3-17 days	half life days
Microbial Degradation	3	
Environmental Partitioning: Fugacity	0.000001714	Pa
Air %	4.15	
Soil %	5.99	
Water %	84.25	
Suspended Solids %	0.01	
Aquatic biota %	0	
Sediment %	5.59	
Bioconcentration factor (BCF)	14.57	

Both bioconcentration factors (BCFs) or bioaccumulation factors (BAFs) are used in assessments. The BCF is usually determined experimentally. The  $k_{ow}$  is generally

used to estimate the BCF of chemicals and good relationships have been identified between the BCF and the  $k_{ow}$  (e.g., Veith et al. 1979, Mackay 1982). However, their relationship is affected by the structure of the chemical. Meylan et al. (1999) have refined the relationship between  $k_{ow}$  and BCF classifying compounds as non-ionic or ionic (the latter group including carboxylic acids, sulfonic acids and their salts and quaternary-N compounds). For non-ionic compounds a series of correction factors are applied depending on the structure of the compound. Different equations are also applied to those compounds with  $k_{ow} > 7.0$ . BCF data is difficult to determine experimentally and a limited amount of BCF data can be obtained from the literature or from databases (for example refer to ECOTOX and also to the USACOE BCF database). The BCF can be estimated for individual chemical species using programmes such as BCFWIN (Syracuse Research Corporation). Calculations of BCF in that programme are made using  $K_{ow}$  and the methodology developed by Meylan et al. (1999). If BCF data are available for more than one species then the highest BCF is utilised.

In terms of environmental significance, USEPA (1985) considered that compounds with  $\log k_{ow}$  values of more than 3.5 should be considered further in relation to bioaccumulation.

## 7 RISK ASSESSMENT

### 7.1 Introduction

In addressing the overall question of what constitutes an environmental risk in relation to a contaminant entering the aquatic environment, the following questions need to be answered:

- What factors determine or constitute defining the potential risk?
- What is the basis for identifying the potential risk?
- What is the implication of identifying a potential risk?

In the Transport Contaminant database screening assessment, the methodology identified in the following sections is utilised for all contaminants put up to the screening process irrespective of the existence of information about the contaminant.

### 7.2 Factors defining risk

In its most simplest form, risk can be defined as:

$$\text{Risk} = \text{Hazard} \times \text{Exposure}$$

This is the definition used both by the USEPA in the New Chemicals Programme and the Australian National Pollutant Inventory (NPI).

In the NPI, hazard is defined as the harm potentially caused by a substance and risk is a measure of the likelihood of harm being caused by a substance. The amount of risk increases with the amount of exposure. Exposure (e.g., in terms of external exposure, the concentration in water or sediment) is dependent on a range of specific factors that influence the actual exposure or dose. These include bioavailability, metabolic transformation and excretion, exposure period and concentration.

In a screening process such as this, exposure information is not available and the screening is performed in the absence of exposure data. The use of exposure data is discussed further in Section 7.5.

In the Transport Contaminant screening process, the core framework factors have been based upon the USEPA P2 Framework and also in part that of the NPI (NPI 1999) and SIDS (OECD 1997). The P2 Framework is used in the PBT Chemicals Initiative (Persistent, Bioaccumulative and Toxic Chemicals).

The core factors used in the Transport Contaminant screening assessment are:

- ❑ Environmental persistence.
- ❑ Bioaccumulation.
- ❑ Toxicity.
- ❑ Bioavailability

The accumulative risk derived from each of these factors determines the overall potential risk associated with the contaminant. This is discussed in more detail in the following section.

## 7.3 Database/Risk factors

### 7.3.1 Introduction

In this section, each of the factors and information presented in the database is identified and the guidance utilised to identify potential risk is identified.

### 7.3.2 Persistence and Fate

Persistence can be assessed and interpreted in a number of ways (e.g., in relation to photo-degradation, stability in water, microbial degradation). Persistence is also covered within the bioavailability factor rank. The following information is presented in the database where available:

- ❑ Hydrolysis half life (ASTER).
- ❑ BOD half life (ASTER).
- ❑ Environmental partitioning (MacKay level 1) at 25°C (ASTER)
- ❑ Biodegradation under aerobic conditions (BIOWIN).

Microbial degradation rate and BOD half life are used to score the overall persistence of the contaminant. Information on hydrolysis has been included in the database but has not been used to provide information for the overall assessment. Hydrolysis can be added but given the indication of the range of hydrolysis values obtained from ASTER, its inclusion would not significantly influence the final degradation score. OECD (1998) identified evidence of rapid hydrolysis being more than 10% in five days (i.e., a hydrolysis half life of more than one year) and rapid biodegradation as significant degradation being achieved within 10 days in a 28 day degradation test. Substances with hydrolysis half lives of less than one day were considered unstable (OECD 1998).

BLOWIN, which was used to assess the probability of microbial degradation (Howard et al. 1992, Boethling et al. 1994), rates the biodegradation probability as “biodegrades fast” and “does not biodegrade fast). This rating is similar to that identified in BLOWIN for the Japanese MITI (Ministry of International Trade and Industry) biodegradation test (Tunkel et al. 2000). Both models utilise linear and non-linear regression. As a result, the models each produce two results and in some cases a chemical may be assessed in both categories of degradation. As such, the predominant degradation probability of both models was used. Where there was an ambivalence in the output, an intermediate score was given.

To accommodate the BLOWIN output in the assessment, microbial biodegradation is ranked as:

Rapid	score 1.
Slow	score 2.
Persistent (does not degrade fast)	score 3.

The estimated BOD half life has been assessed on the basis of:

Rapid (<15 days)	Score 1.
Slow (>15 days but <100 days)	Score 2.
Persistent (>100 days)	Score 3.

This rating is based in part on the OECD definition of rapid degradation and the range encountered in the data-set.

As the majority of the organic compounds are unlikely to undergo hydrolysis this aspect of degradation has not been included in the assessment process as it would have little effect on the overall persistence score. Should a wider range of hydrolysis rates be identified, this factor can be added back into this part of the overall risk assessment.

### 7.3.3 Toxicity

A range of data is usually available in relation to toxicity to aquatic organisms. This data typically varies in relation to the length of exposure and the end-points used to identify toxicity. Both NPI (1999) and OECD (1997) identified toxicity data that could be utilised in toxicity screening. They also identified assessment factors that could be applied to toxicity data to obtain a probable no effects concentrations for chemicals. In this screening assessment, the ranking of toxicity endpoints used by NPI (1999) has been used with minor modification. The database identifies the lowest chronic toxicity data-point and based on the lowest data-point, a factor of 10 is used to identify a preliminary ENEV based upon chronic data. In cases where only acute data is available the CTV is

divided by 100 to produce an ENEV concentration. The single ENEV is used in the assessment score.

For Chronic Toxicity

High toxicity – ENEV <10 mg/m <sup>3</sup>	Score 3.
Medium toxicity – ENEV >10 mg/m <sup>3</sup> and <100 mg/m <sup>3</sup>	Score 2.
Low toxicity – ENEV >100 mg/m <sup>3</sup>	Score 1.

This set of thresholds is lower than the threshold trigger for ecotoxicity identified by ERMA (1999). That threshold is based upon NOEC values (less than or equal to 1000 mg/m<sup>3</sup>). This trigger corresponds more closely to the CTV value identified in the database rather than the ENEV value.

#### 7.3.4 Bioaccumulation

Bioaccumulation is assessed in the screening assessment by calculating the BCF for the contaminant. The database includes data on the  $k_{ow}$  and the BCF which is calculated using the programme BCFWIN. BCFs for fish range from low factors such as o-xylene (50.4), naphthalene (69.34) through to dieldrin (2,871) to DDT (41,750). BCF values have been used to score potential risk in this area via the following ranking:

High risk	BCF >1000	Score 3.
Medium risk	BCF <1000 and >100	Score 2.
Low risk	BCF <100	Score 1.

The BCF cutoffs are based on the primary cutoff defined for identifying bioaccumulating chemicals of concern NPI (1999).

#### 7.3.5 Bioavailability

Bioavailability is a key generic factor that determines the overall exposure of biota to a contaminant. Bioavailability is a relatively complex phenomenon dependent upon a considerable number of specific factors. Data is present in the data-base for several key factors. These include vapour pressure, water solubility and Henry's constant. These have been combined to provide a bioavailability score.

#### 7.3.6 The State

State has three categories, liquid, gas and solid. The scoring has identified liquid as having a specific ranking higher than solid or gas due to liquid" contaminants having a more direct relationship with the water in stormwater and aquatic systems. As solid phase contaminants (e.g., in rubber) may be released over time (e.g., through microbial degradation), this was not considered sufficiently fast to justify setting the score for solid state contaminants as a 2.

Liquid	Score 3.
Solid	Score 1.
Gas	Score 1.

### 7.3.7 Solubility

High solubility typically leads to rapid distribution of the contaminant in aquatic systems. It also means that the contaminant will typically have a low affinity for particulate material and also it typically infers relatively rapid degradation. Solubility varies orders of magnitude between contaminants. For example hexachlorobenzene has a solubility at 25 °C of 0.006 g/m<sup>3</sup>; naphthalene 13 g/m<sup>3</sup>; benzene 1,800 g/m<sup>3</sup>; MTBE 48,000 g/m<sup>3</sup>. To provide a relative ranking of solubility the following rank scores were identified:

Insoluble or slightly soluble (< 1,000 g/m <sup>3</sup> )	Score 1.
Moderate solubility (>1,000-<10,000 g/m <sup>3</sup> )	Score 2.
Highly soluble (> 10,000g/m <sup>3</sup> )	Score 3.

### 7.3.8 Vapour Pressure

Vapour pressure strongly influences environmental partitioning (especially between air and water). VP at 25 °C ranges considerably between compounds. For example 0.09 mm Hg for naphthalene; 95 mm Hg for benzene to 249 mm Hg for MTBE. The following VP values were used to rank VP values.

Stable or very low vapour pressure (< 1 mm Hg)	Score 3.
Moderate vapour pressure (>1-<100 mm Hg)	Score 2.
High vapour pressure (>100 mm Hg)	Score 1.

### 7.3.9 Henry's Law Constant

Henry's Law constant is a measure of the ability of an organic compound to volatilise. Lyman et al. (1982) define Henry's constant ranges in relation to degree of volatility and these have been used as the basis of the scoring in the contaminant assessment.

Non volatile (< 3 x 10 <sup>-7</sup> atm-m <sup>3</sup> /mole)	Score 3.
Intermediate (> 3 x 10 <sup>-7</sup> to < 10 <sup>-3</sup> atm-m <sup>3</sup> /mole)	Score 2.
Rapid volatilisation (> 10 <sup>-3</sup> atm-m <sup>3</sup> /mole)	Score 1.

Those chemicals which exist essentially in the gas phase were scored as 1.

The four scores from the bioavailability factors are combined and divided by four then rounded to the nearest whole number to provide a bioavailability score.

## 7.4 Identification of Potential Risk

The purpose of this process is to identify whether a contaminant is a Contaminant of Potential Concern (COPC). As identified in the database, there is a range of contaminants emitted by motor vehicles (or rail locomotives etc) that have already been identified as COPCs by virtue that they have already have environmental guideline values for sediments or water. In the case of these contaminants, the label of COPC only changes to a Contaminant of Concern (COC) if the guidance value is exceeded.

To be identified as a COPC through this assessment process, a contaminant has to have characteristics that identify it as persistent, bioaccumulative or toxic and bioavailable as defined in the earlier sections. The overall assessment is carried out via a ranking and sum of rank values.

In the NPI (1999) chemicals ranking process, the approach to identifying overall risk was discussed and recognised that there are issues and difficulties with any approach adopted. NPI (1999) eventually adopted a single score for health and environment which when multiplied by the exposure score (i.e.,  $\text{risk} = \text{exposure} \times \text{effect or hazard}$ ) produced a risk score with a range 0 – 18. NPI (1999) opted to include any chemical with a score over 3 on the National Pollutant List. Cardwell et al. (1983) presents information on the identification of COCPs. In the transport contaminant assessment process, Hazard Quotients based upon the environmental concentration cannot be used as in a preliminary screening process as the concentration data for the individual contaminants may not be available.

The following procedure was utilised to identify a contaminant as a COPC.

1. The score for persistence was identified (1-3).
2. The score for bioaccumulation was identified from calculation of the BCF (1-3).
3. The toxicity was assessed through estimation of the ENEV (based upon chronic toxicity) and given a score ranging from 1-3.
4. Bioavailability was assessed by assessing the form and bioavailability in aquatic systems (via presence in water).

The scores are then multiplied together to provide a score in the range 1 ( $1 \times 1 \times 1 \times 1$ ) to 81 ( $3 \times 3 \times 3 \times 3$ ). Any contaminant with a score of over 8 is identified as a contaminant of concern. A score of 8 represents at least three of four of the key factors having a moderate P, B or T. Table 6.1 provides a summary of the aquatic risk score calculation matrix. A screen shot from the final summary screen in the database is shown below.

Properties		Toxicity		Persistence and Bioaccumulation	
Risk		Regulatory - Sediment		Regulatory - Water	
Bioavailability:	State	<input type="text" value="3"/>			
	Solubility	<input type="text" value="1"/>			
	VP	<input type="text" value="3"/>			
	HLC	<input type="text" value="2"/>			
	Overall score		<input type="text" value="2.25"/>		
Persistence:	Microbial Deg	<input type="text" value="2"/>			
	BOD Half Life	<input type="text" value="1"/>			
	Overall score		<input type="text" value="1.50"/>		
Toxicity:			<input type="text" value="3"/>		
Bioaccumulation:			<input type="text" value="1"/>		
				<b>Overall Risk</b>	<input type="text" value="10.13"/>

**Table 6.1 - Summary of Aquatic Risk Score Calculation**

Category	Factor		Score	Category Score	Overall Score
				<u>Factor Score</u> Number of factors	1x2x3x4
1. Bioavailability	1.1	State	√	-	-
	1.2	Solubility	√	-	-
	1.3	VP	√	-	-
	1.4	HLC	√	-	-
				√	-
2. Persistence	2.1	Micro Degradation	√	-	-
	2.2	BOD half life	√	-	-
				√	-
3. Toxicity	3.1	ENEV	√	-	-
				√	-
4. Bioaccumulation	4.1		√	-	-
		BCF			
				√	-
					√

## 7.5 Follow Up

The key question which arises following the identification of a COPC is what does the identification as a COPC mean?

In the context of the screening process, it is a step in the evaluation process. It provides a mechanism to flag the presence of a contaminant for further consideration. It does not mean that the presence constitutes an environmental risk.

Following identification of a contaminant as a COPC, the following steps can be taken.

1. Confirm the source/route of exposure.
2. Identify the amount of contaminant emitted.
3. Identify the concentration of the contaminant of concern in the aquatic compartment of interest.

The evaluation of exposure can be assessed at three levels:

NPI (1999) identified a simple exposure assessment process as part of the identification of chemicals for the Australian NPI. Based upon the NPI process, the following exposure ranking can be utilised to carry out an initial refinement of the COPC identification. Release from vehicles:

Widespread use and release	Score 3.
Moderate use and release	Score 2.
Minor use and release	Score 1.

Any COPC scoring 1 in the source and release ranking would be potentially scaled down as a COPC.

For further evaluation, data on actual release is required. This can be measured or calculated based upon loads and equilibrium partitioning models (e.g., MacKay Level 1 model or more sophisticated). Based upon this data, a preliminary (hypothetical) assessment of contaminant concentration within a given receiving environment can be calculated (using a simple box type model), (refer Cowan et al 1995). This concentration is compared to an assessed NOEC or ENEV. Contaminants with waterborne concentrations above the NOEC or ENEV would confirm their status as COPC.

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### **Addendum Note (June 2004)**

Since this report was prepared, there has been a large number of research papers prepared on the assessment of the environmental significance of unknown compounds using QSARS.

ERMA (<http://www.ermanz.govt.nz/>) provides information on the use and manufacture of hazardous substances in New Zealand. The site also provides internet links to a variety of databases and information on chemicals and toxicity.

Since the development of the vehicle emissions compound database, USEPA has released an updated version of the ECOTOX (<http://www.epa.gov/ecotox/>) and has released a public version of the EPISUITE collection of software that was used to undertake the vehicle contaminant assessments described in this document (<http://www.epa.gov/oppt/exposure/docs/episuite.htm>).

## APPENDIX A

**Table A1 – Summary of key road vehicle contaminant sources and their source codes.**

Powertrain Area	Component	Source Code
Fuel	Base stocks (Petrol)	1.1a
	Base Stock (Diesel)	1.1b
	Blendstocks	1.2
	Additives – initial formulation	1.3
	Additives – after-market	1.4
	Evaporative emissions/leakage	1.5
Exhaust System	Combustion emissions; gaseous,	2.1a
	Combustion emissions; particulate – petrol diesel	2.1b
	Emissions control system; erosion	2.2
	Emissions control system; control additives	2.3
Lubricants	Engine oil	3.1
	Gear oil	3.2
	Bearing grease	3.3
	Chassis grease	3.4
Coolants	Engine coolant	4.1
	Induction intercooler systems	4.2
	Air conditioning	4.3
Sealants	Gaskets	5.1
	Jointing compounds	5.2
	Fillers	5.3
Hydraulics	Brake systems	6.1
	Clutch systems	6.2
	Auto transmission	6.3
	Power transmission	6.4
	Suspension systems	6.6
	Auxiliaries (power transmission)	6.7
Braking (and clutch)	Friction linings	7.1
Tyres	Tread surfaces wear	8.1
	Carcase weathering	8.2
Roads	Pavement surface wear	9.1
	Pavement surfaces; weathering	9.2
Vehicle Body	Plasticisers	10.1
	Paintwork	10.2
	Metal corrosion	10.3
	Surface coatings weathering; (paintwork and underbody protection)	10.4
	Windscreen washer additives	10.5
	Vehicle washdown (roadside)	10.6
	Drive belts; engine auxiliaries	10.7

**Table A2 - Summary of key rail contaminant sources and their source codes.**

<b>Powertrain Area</b>	<b>Component</b>	<b>Source Code</b>
Fuel	Base stocks (Diesel)	1.1b
	Blendstocks	1.2
	Additives – initial formulation	1.3
	Additives – after-market	1.4
	Evaporative emissions/leakage	1.5
Exhaust System	Combustion emissions; gaseous,	2.1b
	Combustion emissions; particulate	2.2
	Emissions control system; erosion	2.3
	Emissions control system; control additives	2.4
		2.5
Lubricants	Engine oil	3.1
	Gear oil	3.2
	Bearing grease	3.3
	Chassis grease	3.4
Coolants	Engine coolant	4.1
	Induction intercooler systems	4.2
	Air conditioning and refrigeration	4.3
Sealants	Gaskets	5.1
	Jointing compounds	5.2
	Fillers	5.3
Braking (and clutch)	Brake shoes	7.1
Wheels	Wheel wear	8.1
Tracks	Track lubrication	9.1
	Points lubrication	9.2
	Sleepers	9.3
Rolling Stock	Cleaning	10.1