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Series

Environmental Assessments of Priority Substances Under the Canadian Environmental Protection Act

Guidance Manual Version 1.0
March 1997

EPS/2/CC/3E
Chemicals Evaluation Division
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Review Notice

The contents of this report have been reviewed by the Chemicals Evaluation Division, Environment Canada and approved for publication. Mention of trade names or commercial products does not constitute recommendation or endorsement for use.

Preface

This manual provides guidance for conducting environmental assessments of priority substances in Canada. It was developed by the Chemicals Evaluation Division, Commercial Chemicals Evaluation Branch, Environment Canada, to update the unpublished document *Draft Guidelines for Conducting Environmental Assessments of Priority Substances Under the* Canadian Environmental Protection Act, *April 1992*. This revision is based on experience gained from assessing substances on the first Priority Substances List and also reflects recent advances in the field of ecological risk assessment. This guidance manual has been extensively reviewed by numerous experts from other government departments, industry, academia, and nongovernmental and international organizations.

The intended audience for this manual is the assessors leading the environmental assessments of priority substances and the groups of experts who will assist them. The secondary audience is those interested parties who wish to gain insight into how Environment Canada conducts environmental assessments of priority substances.

This guidance manual represents the experience gained by the Priority Substances Assessment Program at this time and the current scientific understanding of ecological risk assessment. As more experience is gained during application of the guidance in assessments of substances on the second Priority Substances List, and as the science of ecological risk assessment becomes more developed, the guidance manual will be updated to reflect that experience and knowledge. The manual is intended to provide guidance only, not strict rules, to allow for the flexibility required to assess different types of substances and for developments in experience and science.

This manual is published in both English and French and is available on Environment Canada's Green Lane on the World Wide Web at http://www.ec.gc.ca.

A companion document (*Environmental Assessments of Priority Substances Under the* Canadian Environmental Protection Act — *Resource Document*) elaborates on the guidance provided in this manual and describes methods and approaches in more detail. The resource document is unpublished, but it is available from the Commercial Chemicals Evaluation Branch. Owing to resource constraints, it has not been as thoroughly updated following the review phases as was the guidance manual. A policy and process document that presents guidance on nonscientific issues related to the assessment of priority substances is also available on request from the Commercial Chemicals Evaluation Branch.

Préface

Le présent guide fournit des conseils sur l'évaluation environnementale des substances d'intérêt prioritaire au Canada. Il a été rédigé par la Division de l'évaluation des produits chimiques, Direction de l'évaluation des produits chimiques commerciaux, Environnement Canada, afin de mettre à jour le document non publié *Draft Guidelines for Conducting Environmental Assessments of Priority Substances Under the* Canadian Environmental Protection Act, *April 1992*. Cette révision est fondée sur l'expérience acquise à la suite de l'évaluation des substances figurant sur la première liste d'intérêt prioritaire et tient également compte des récents progrès accomplis dans le domaine de l'évaluation des risques écologiques. Le guide a fait l'objet d'un examen approfondi par de nombreux experts d'autres ministères gouvernementaux, de l'industrie, du milieu universitaire ainsi que d'organisations non gouvernementales et internationales.

Le guide s'adresse tout d'abord aux évaluateurs qui dirigent l'évaluation environnementale des substances d'intérêt prioritaire ainsi qu'aux groupes d'experts qui les aident, puis, en deuxième lieu, aux parties intéressées qui désirent savoir comment Environnement Canada effectue l'évaluation environnementale de ces substances.

Le guide est provisoire parce qu'il reflète l'expérience acquise jusqu'à présent grâce au Programme d'évaluation des substances d'intérêt prioritaire et les connaissances scientifiques actuelles en matière d'évaluation des risques écologiques. Il sera mis à jour pour tenir compte de l'expérience accrue par les conseils qu'il fournit concernant l'évaluation des substances figurant sur la deuxième liste d'intérêt prioritaire et par le perfectionnement des connaissances scientifiques en matière d'évaluation des risques écologiques. Plutôt que d'énoncer des règles rigoureuses, le guide offre des conseils seulement afin d'accorder la souplesse nécessaire pour évaluer différents types de substances et de tenir compte de l'accroissement de l'expérience et des connaissances scientifiques.

Le guide est publié en français et en anglais; il peut aussi être consulté sur la Voie verte d'Environnement Canada qui se trouve sur le site Web et dont l'adresse est http://www.ec.gc.ca.

Un document d'accompagnement (*Environmental Assessments of Priority Substances Under the* Canadian Environmental Protection Act *Resource Document*) étoffe les conseils présentés dans le guide et décrit plus en détail les méthodes et les façons de procéder. Ce document n'a pas été publié, mais il est possible de l'obtenir à la Direction de l'évaluation des produits chimiques commerciaux. En raison de restrictions financières, sa mise à jour, à la suite des diverses étapes de l'examen, n'a pas été aussi complète que dans le cas du guide. La Direction de l'évaluation des produits chimiques commerciaux peut aussi fournir sur demande un document d'orientation et de marche à suivre qui donne des conseils sur les questions non scientifiques se rapportant à l'évaluation des substances d'intérêt prioritaire.

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LIST OF ACRONYMS

ACR	Acute/chronic ratio
AET	Apparent effects threshold
ANOVA	Analysis of variance
AOX	Adsorbable organic halogen
ASTM	American Society for Testing and Materials
BACI	Before–After–Control–Impact
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
CAS	Chemical Abstracts Service
CBB	Critical body burden
CCME	Canadian Council of Ministers of the Environment
CDF	Cumulative density function
CEARC	Canadian Environmental Assessment Research Council
CEPA	*Canadian Environmental Protection Act*
CEU	Commission of the European Union
CFC	Chlorofluorocarbon
CTV	Critical toxicity value
DOC	Dissolved organic carbon
EC_{50}	Median effective concentration
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
EC_x	Effective concentration for an x% effect
EEV	Estimated exposure value
ENEV	Estimated no-effects value
EqP	Equilibrium partitioning
FETAX	Frog embryo teratogenesis assay
GIS	Geographic information system
GWP	Global warming potential
IBI	Integrated Biotic Index
IC_{25}	Inhibiting concentration for a 25% effect
IC_p	Inhibiting concentration for a p% effect
IR	Infrared
IUPAC	International Union of Pure and Applied Chemistry
K_{oc}	Organic carbon partitioning coefficient
K_{ow}	Octanol–water partition coefficient
LC_{50}	Median lethal concentration
LD_{50}	Median lethal dose
LOEC	Lowest-observed-effects concentration
LOEL	Lowest-observed-effects level
MATC	Maximum allowable toxicant concentration
MIR	Maximum incremental reactivity
MMWG	Metals and Minerals Working Group
MOIR	Maximum ozone incremental reactivity
mRNA	Mitochondrial ribonucleic acid
NOEC	No-observed-effects concentration
NOEL	No-observed-effects level
OC	Organic carbon
ODP	Ozone-depleting potential
OECD	Organisation for Economic Co-operation and Development
OFP	Ozone-forming potential
OM	Organic matter
PAH	Polycyclic aromatic hydrocarbon
PCB	Polychlorinated biphenyl
PDF	Probability density function
POCP	Photochemical ozone creation potential
PSL	Priority Substances List
QA/QC	Quality assurance/quality control
QSAR	Quantitative structure–activity relationship
RBE	Relative biological effectiveness
RIVM	The Netherlands National Institute of Public Health and Environmental Protection
SETAC	Society of Environmental Toxicology and Chemistry
TEF	Toxic equivalent factor
TIE	Toxicity identification and evaluation
TU	Toxic unit
U.S. EPA	United States Environmental Protection Agency
VKI	Water Quality Institute (Denmark)
VOC	Volatile organic compound
WCEM	Wildlife Contaminant Exposure Model
WCO	Waste crankcase oil
WERF	Water Environmental Research Foundation

Glossary

Absorption: The penetration of one substance into the inner structure of another.

Acute/chronic ratio: A species' mean acute value divided by the chronic value for the same species. Such ratios can be used to convert the median lethal results of a short-term study to an estimated long-term no-effects concentration.

Acute toxicity test: A toxicity test of short duration in relation to the life span of the test organism (e.g., usually ≤ 4 days for fish).

Adsorption: Adherence of the atoms, ions, or molecules of a liquid or gas to the surface of another substance.

Alpha (α): The symbol for a Type I error in hypothesis testing, expressed as a probability or proportion (e.g., 0.05 or 5%). A Type I error is the probability of rejecting the null hypothesis when in fact the null hypothesis is true. In hypothesis testing, α is specified by the user prior to carrying out the analysis (see *Beta*).

Atmospheric lifetime (or natural lifetime, J): The time it takes for the reactant concentration to fall to 1/e of its initial value (e is the base of natural logarithms, 2.718), or 36.7% of the original concentration. The lifetime is related to the rate constant and to the concentrations of any other reactants involved in the reactions.

Benthic organism: An organism that lives in or on the bottom of a body of water.

Beta (β): The symbol for a Type II error in hypothesis testing, expressed as a probability or proportion. A Type II error is the probability of accepting the null hypothesis when in fact the null hypothesis is false. The magnitude of the Type II error is generally inversely related to the magnitude of the Type I error that will be tolerated (see *Alpha*).

Bioaccumulation: The net accumulation of a substance by an organism as a result of uptake from all routes of exposure.

Bioaccumulation factor (BAF): The ratio of the steady-state concentration of a substance in an organism owing to uptake from all routes of exposure to the concentration of the substance in the medium to which the organism was exposed.

Bioavailable substance: A substance that is present in a form that can be readily taken up by exposed organisms.

Bioconcentration: The net accumulation of a substance directly from aqueous solution by an aquatic organism.

Bioconcentration factor (BCF): The ratio of the steady-state concentration of a substance in an organism owing to uptake via contact with water to the concentration of the substance in the test water; and/or the ratio of the uptake rate constant to the depuration constant, assuming first-order kinetics.

Biotransformation: A process mediated by microorganisms or other living organisms that chemically alters the structure of a chemical.

Body burden: The amount of a substance that has accumulated in the tissue of an exposed organism, usually expressed as the concentration of the substance in a particular organ or in the whole organism.

Carrier and noncarrier controls: Toxicity tests for certain substances may use a carrier to aid in dispersing the test substance evenly in the test medium. Carrier and noncarrier controls are conducted with and without the carrier, respectively, in order to determine the effects of the carrier on the test organisms.

Chronic toxicity test: A toxicity test that spans a significant portion of the life span of the test organism (e.g., 10% or more) and examines effects on such parameters as metabolism, growth, reproduction, and survival.

Complex: Dissolved species formed from two or more simpler species, each of which can exist in aqueous solution.

Complex substance: Consists of a heterogeneous association of many substances (i.e., constituents) that are not necessarily related and either are released at a given time and place or occur at a given time and place; see definitions of *Mixture* and *Effluent*.

Critical body burden (CBB): The minimum concentration of a substance that causes an adverse effect on the measurement endpoint (e.g., reproductive potential of *Daphnia*) of interest.

Critical toxicity value (CTV): The quantitative expression (e.g., IC_{25}) of low toxic effect on the measurement endpoint. CTVs are used in risk characterization for the calculation of an estimated no-effects value (ENEV).

Cumulative probability distribution: A curve or mathematical expression that quantifies uncertainty over a variable. It associates a probability with all values in the set of possible values. The probability associated with each value of the variable is that of the occurrence of a value less than or equal to the specified value.

Depuration: Clearance of a chemical from an organism as a result of elimination and/or degradation.

Desorption: The removal of an adsorbed material from the substance on which it is adsorbed.

Detritivore: An organism that feeds primarily on detritus (i.e., organic particulate matter from nonliving and decomposing organisms).

EC_x: The concentration of a substance that is estimated to cause some toxic effect on x% of the test organisms. The duration of the exposure must be specified. EC_x describes quantal effects, lethal or sublethal, and is not applicable to quantitative effects (see IC_p).

Ecological risk assessment review group: A group of risk assessors, risk managers, and other interested parties who will review the problem formulation stage and data gaps and recommend research priorities for PSL2 substances.

Effluent: A liquid complex substance composed of many constituents that are not necessarily related, that emerge from a pipe or similar outlet, and that are discharged primarily into aquatic systems (e.g., industrial discharge, sewage effluent).

Elutriate: An aqueous solution obtained by adding water to a solid substance (e.g., sediment, tailings, drilling mud, dredge spoil), shaking the mixture, then centrifuging or filtering it or decanting the supernatant.

Endocrine disrupter: A substance that interferes with the production, release, transport, metabolism, binding, action, or elimination of natural ligands in the body that are responsible for the maintenance of homeostasis and the regulation of developmental processes.

Environmental resource group: A group of people drawn from government, the private sector, and academia who will assist with the conduct and review of the ecological risk assessment of a substance.

Equilibrium: A condition in which the ratio of the concentrations of a substance in two or more phases (e.g., pore water and particulate phases of bottom sediments) is constant.

Food web structure: Consists of many interlinked food chains (i.e., organisms forming a series through which energy is passed). A typical food chain structure consists of producer (e.g., green plant)→ primary consumer (e.g., herbivore)→ secondary consumers (consisting of smaller then, at subsequent trophic levels, larger carnivores).

Fugacity: The thermodynamic or "escaping tendency" of a chemical in a particular phase (e.g., water, air), given in units of partial pressure or pascals (Pa). If the fugacity of a chemical is higher in water than in air, the chemical will evaporate until an equilibrium is established.

Genotoxicity: The ability of a substance to damage the genetic material of an organism, which is then passed on to the next generation.

Group parameter: Group parameters are based on analytical-chemical techniques and determine specific elements or chemically defined groups of constituents in complex substances. Examples of group parameters are dissolved organic carbon (DOC) and Adsorbable Organic Halogen (AOX).

Hydrolysis reaction: For organic substances, a reaction involving the introduction of a water molecule or a hydroxyl ion into an organic molecule, resulting in the cleavage of a chemical bond in the organic molecule. For inorganic substances, a reaction involving a water molecule and an inorganic substance, resulting in the cleavage of the water molecule.

IC_p: The inhibiting concentration for a specified percent effect. A point estimate of the concentration of a test substance that causes p% reduction in a quantitative biological measurement such as growth rate.

Immune suppression: The suppression of the reaction of the immune system by a substance, which leaves the organism vulnerable to infection, disease, etc.

Interpolation: The process of estimating a value between two or more known values.

LC_{50}: The concentration of a substance that is estimated to be lethal to 50% of the test organisms over a specified period of time.

LD_{50}: The dose that causes mortality in 50% of the organisms tested.

LOEL: Lowest-observed-effect level. The lowest concentration or dose in a toxicity test that causes a statistically significant effect in comparison to the controls.

MATC: The maximum allowable toxicant concentration, generally presented as the range between the NOEL and LOEL or as the geometric mean of the two measures.

Mean: The arithmetic average of a set of numerical observations, calculated as the sum of the observations divided by the number of observations.

Mesocosm: A small-scale model ecosystem somewhat similar to a microcosm (see *Microcosm*), but larger. Mesocosms are often artificially constructed outdoor ponds with a volume of 100–1000 m^3.

Microcosm: A small-scale model ecosystem, often contained in a laboratory test chamber, to which the test chemical is added. A microcosm typically contains more than one phase (e.g., water, sediment, and biota).

Mineralization: Breakdown of an organic substance to form carbon dioxide, water, nitrate, and phosphate ions.

Mixture: A liquid, solid, or gaseous complex substance composed of many constituents that are not necessarily related and are released into various environmental compartments, including water, air, and land (e.g., waste crankcase oils, creosote-impregnated waste materials, landfill leachate, smelter emissions).

Mode of action: The manner in which a substance causes an adverse effect in an organism (e.g., narcosis, acetylcholinesterase inhibition, central nervous system seizure).

Narcotic substance: Any substance that induces narcosis (i.e., a reversible state of stupor, insensibility, or unconsciousness) in an organism. The mechanism of narcosis is nonspecific, and, consequently, a narcotic substance's toxicity is entirely dependent on its tendency to partition to the tissue of the organism.

NOEL: No-observed-effect level. The highest concentration or dose in a toxicity test not causing a statistically significant effect compared with the controls.

Nutrient cycling: The dissipation of energy in ecosystems through the transport, decomposition, and recycling of materials bound up in the biomass, living or dead, of system components. Nutrient cycling can often be constrained by the availability to primary producers of essential raw materials, including macronutrients (e.g., phosphorus, nitrogen, calcium) and trace nutrients (e.g., iron, manganese, molybdenum).

Pelagic biota: Aquatic organisms living in the water column of a body of water, rather than along the shore or in the bottom sediments.

Photolysis (direct): The decomposition or reaction of a substance on exposure to light. Occurs when sunlight is absorbed by a substance and the energy is used to form excited or radical species, which react further to form stable products.

Photolysis (indirect, or photooxidation): The reaction of a substance with intermediate oxidants formed during photolysis of dissolved organic matter in water or soil, or photolysis of ozone or nitrogen dioxide in the atmosphere.

Photosynthesis: The elaboration of organic matter (carbohydrate) from carbon dioxide and water with the aid of light energy.

Pore water: Water occupying the space between sediment particles. The amount of pore water is expressed as a percentage of the wet sediment, by weight.

Probability density function: A probability distribution describing a continuous random variable. It associates a relative likelihood to the continuum of possibilities.

Radiative balance: The quasi-equilibrium between the heat absorbed by the Earth from the sun and the heat lost by the Earth through radiation.

Receptor: In this document, "receptor" refers to any environmental entity that is exposed to, and could be adversely affected by, a PSL substance. A receptor is usually an organism or a population, but it could also be an abiotic entity, such as stratospheric ozone.

Regression analysis: A statistical procedure based on empirical data that determines the coefficients in a linear or nonlinear combination of one or more independent variables that best estimates the value of a dependent variable.

Saprovore: An organism that feeds primarily on dead or decaying organic matter.

Sediment: Natural particulate matter that has been transported to, and deposited at, the bottom of a body of water. The term can also describe a substrate that has been experimentally prepared and into which test organisms can burrow.

Sensitivity analysis: The computation of an output distribution's sensitivity with respect to the input probability distributions.

Solid-phase sediment: The whole, intact sediment rather than a derivative of the sediment, such as an elutriate or a resuspended sediment.

Sorption: A surface phenomenon that may be either absorption or adsorption, or a combination of the two.

Spiked sediment: A control, reference, or other clean sediment to which a test substance (such as a chemical or mixture of chemicals) has been added, then mixed throughout the sediment.

Spiked-sediment toxicity test: An assay using a test organism that is exposed to specified concentrations of a substance-spiked sediment over a specified time period to determine any effects.

Standard deviation: A measurement of the variability of a distribution. The standard deviation is the square root of the variance.

Steady-state concentration: A condition in which the concentration of a substance in a particular medium is constant.

Sublethal toxicity test: A toxicity test conducted using concentrations or doses of a substance below levels causing death within the test period. Common endpoints for sublethal toxicity tests include reduction in growth or number of young produced.

Vapour pressure: The pressure exerted by the vapour phase of a substance when it is in equilibrium with the liquid or solid form from which it is derived. Vapour pressure may be considered a measure of a pure substance's tendency to volatilize.

Variance: A measure of the dispersion, or spread, of a set of values about a mean. When values are close to the mean, the variance is small. When values are widely scattered about the mean, the variance is larger. Variance is the mean of the squares of the deviations from the mean of the distribution.

Volatilization: The transfer of a substance from a liquid or solid to a vapour phase.

Water hardness: The amount of calcium and magnesium carbonates, bicarbonates, sulphates, and chlorides contained in a given amount of water. Water hardness is usually expressed as the equivalent quantity of calcium carbonate. Water containing less than about 85 mg calcium carbonate per litre is considered to be soft, whereas water containing more than about 500 mg calcium carbonate per litre is considered to be very hard.

Chapter 1
Framework and Overview

1.1 Legislative Framework

The *Canadian Environmental Protection Act* (CEPA), proclaimed by the Government of Canada in 1988, provides a legislative framework to deal with toxic substances in the environment. The Act, administered by Environment Canada and Health Canada, emphasizes prevention and deals with all stages of a substance's life cycle, from research and development to manufacture, transportation, distribution, use, and disposal.

The Priority Substances Assessment Program is mandated under Section 12 of the Act. That Section instructs the Ministers of Environment and Health to develop a list of substances that should be given priority for assessment to determine whether they are "toxic", as defined under Section 11 of the Act. Section 11 states:

> *"A substance is toxic if it is entering or may enter the environment in a quantity or a concentration or under conditions*
>
> *(a) having or that may have an immediate or long-term harmful effect on the environment;*
>
> *(b) constituting or that may constitute a danger to the environment on which human life depends; or*
>
> (c) constituting or that may constitute a danger in Canada to human life or health."

If the assessment concludes that a priority substance is "toxic" under the Act, the substance enters the risk management phase. Management strategies for "toxic" substances are currently being developed through a multistakeholder Strategic Options Process that considers such things as the sources, release rates, and potential effects; existing pollution control technologies; and target markets and impact on competitiveness. Risk management options can include voluntary controls, process changes, substitutions, economic measures, federal regulations, guidelines or codes of practice, control by other federal or provincial/territorial legislation, or a combination of these measures.

The first Priority Substances List (PSL1), which appeared in the *Canada Gazette* in February 1989, contained 44 substances, including organic compounds, metals, mixtures, effluents, and emissions. Assessments of these substances were completed by February 1994. The Ministers of Environment and Health established a second Expert Advisory Panel in December 1994 to recommend a new list of priority substances for assessment under the Act. This Panel, drawn from major stakeholder groups, recommended a list of 25 substances (Ministers' Expert Advisory Panel 1995). The Ministers accepted this list and published the second Priority Substances List (PSL2) in the *Canada Gazette* on December 16, 1995 (Box 1.1).

Box 1.1 Second Priority Substances List*

Acetaldehyde
Acrolein
Acrylonitrile
Aluminum chloride, aluminum nitrate, aluminum sulphate
Ammonium in the aquatic environment
1,3-Butadiene
Butylbenzylphthalate (BBP)
Carbon disulphide
Chloramines
Chloroform
N,N-Dimethylformamide (DMF)
Ethylene glycol
Ethylene oxide
Formaldehyde
Hexachlorobutadiene (HCBD)
2-Methoxy ethanol, 2-Ethoxy ethanol, 2-Butoxy ethanol
N-Nitrosodimethylamine (NDMA)
Nonylphenol and its ethoxylates
Phenol
Releases from primary and secondary copper smelters and copper refineries
Releases from primary and secondary zinc smelters and zinc refineries
Releases of radionuclides from nuclear facilities (impacts on nonhuman species)
Respirable particulate matter less than or equal to 10 micrometres in diameter
Road salts
Textile mill effluents

*See Expert Advisory Panel report for details on how substances were selected (Ministers' Expert Advisory Panel 1995).

1.2 What Are We Trying to Protect?

The objective of the environmental assessment is to determine whether the substance is "toxic" as defined in CEPA Section 11 and to provide scientific support for the determination. To determine whether or not a substance is CEPA "toxic," the assessment estimates and describes risks to receptors (e.g., plants, animals) exposed in the Canadian environment.

Environmental assessments can be complex. They must consider numerous species that may be affected by a substance, either directly or indirectly due to disruptions to ecosystem structure and function. Given our limited understanding of ecosystem structure and function and the scarcity of information typically available, assessors must carefully consider which effects are potentially ecologically significant. Several factors affecting this judgment are discussed in the following Section.

1.2.1 Levels of Biological Organization

Effects in the environment resulting from exposure to chemical substances can occur at various levels of biological organization. Effects at lower levels, such as biochemical effects, are not always transmitted to higher levels, such as ecosystems (Allen and Starr 1982; O'Neill *et al.* 1986). Conversely, in cases in which effects at higher levels have occurred, lower levels of organization will also have been seriously affected (Allen and Starr 1982; O'Neill *et al.* 1986). Therefore, effects observed at the population, community, or ecosystem level are generally considered more environmentally harmful and are of more concern than those observed only at lower levels. Effects on the individual may be significant for threatened or endangered species, where population levels are low.

Few studies have directly tested priority substances for effects at the population, community, or

ecosystem level of organization. Most toxicity studies are conducted in the laboratory using relatively small sample sizes relative to population sizes in natural communities. However, many of the effects measured in laboratory and field studies have implications for populations, communities, and ecosystems. Effects such as endocrine disruption, lethality, and reproductive impairment are closely related to the viability of natural populations. A strong link between toxicity study results (e.g., reduction in reproductive fecundity) and environmental parameters (e.g., population age structure) can provide good evidence for determining whether a substance is "toxic" as defined in CEPA. It is impossible to specify a rigid cutoff point at which effects are considered sufficient to declare the substance "toxic". Professional judgment is required. The following examples illustrate how such judgment may be applied.

- Based on a pathways analysis for chemical A, richness and abundance of grain-eating birds have been selected as the assessment endpoints (see Section 3.6 for a discussion about this term). No field surveys or tests have been conducted to determine whether community-level endpoints have been affected in areas where the chemical has been released. Available information indicates that the chemical is acutely toxic to chickens in laboratory tests at exposure levels similar to those predicted for wild birds, and, further, dead birds have been reported following releases of the chemical. Although these measurement endpoints (see Section 3.7) are at the individual level, one can reasonably argue that the evidence suggests a potential for adverse effects on the assessment endpoint. This evidence could therefore indicate that chemical A is "toxic" under CEPA. It is not possible to prove that adverse effects will occur or to determine the ecological consequences of such effects. Many factors could enhance or mitigate the translation of effects from the individual to community level of organization. For example, if the birds are undernourished in the field, adverse effects predicted by laboratory studies on well-fed birds may considerably underestimate true risk. Conversely, if population size is regulated by recruitment from uncontaminated populations elsewhere, risks predicted by the laboratory test results alone will overestimate true risk (Underwood 1995).

- The assessment endpoint for chemical B is abundance of salmonids based on evidence that the chemical is water soluble and is released to water bodies inhabited by these fish. Chemical B is an estrogen agonist that persists in the environment. Laboratory evidence shows that it competitively binds to the estrogen receptor, thus blocking binding by endogenous 17ß-estradiol, estrone, and estriol; it causes estrogen-inducible responses *in vitro* in fish cells and *in vivo* in rats (example adapted from Kramer and Giesy 1995). Further, levels of the chemical are highest during periods of low steroid biosynthesis in salmonids, such as during male embryo development. This increases the relative potency of exogenous chemical B relative to the endogenous estrogens. Finally, there have been anecdotal observations of hermaphroditic fish downstream of wastewater treatment plants releasing chemical B. Field studies in areas heavily contaminated by other estrogen agonists show that observed effects at the biochemical and physiological levels can be translated into serious adverse effects at the population level owing to declines in reproductive success (Fry *et al.* 1987). This evidence indicates that chemical B is "toxic" as defined under CEPA.

- The assessment endpoint for chemical C, which is released periodically to trout streams, is abundance of salmonids. The chemical is not considered to be persistent. At levels found downstream from outfalls following its release, induction of cytochrome P450 mRNA and P450 protein in rainbow trout has been observed within 18 hours of the initial exposure. The levels of mRNA in chemical C-treated fish peaked at about two days and decayed by five days; P450 protein levels remained elevated somewhat longer but declined to control levels at about 10 days. Corresponding acute and chronic toxicity studies indicate that trout survival, growth, and reproduction were not affected at similar levels of chemical C following a single-dose treatment. Given that chemical C is released

only periodically, that it is not persistent, and that its effects at the biochemical level do not appear to translate to effects at higher levels, the evidence suggests that this chemical would not be considered "toxic" as defined under CEPA based on this particular biochemical level effect.

1.3 Beyond "Toxic"

Although Section 11 of CEPA requires only a determination of whether a substance is "toxic", Section 13 requires that a summary of the assessment be published in the *Canada Gazette*, including a statement of whether the Ministers intend to recommend that regulations be made with respect to the substance. This means that the PSL assessment must include adequate information for risk management decisions. Therefore, where a substance is toxic, the risk assessment should, when possible, include detailed characterization of the substance's entry into the Canadian environment and specify the probabilities and magnitudes of environmental effects at sites of elevated exposure in Canada. Such information is useful in determining the priority for risk management actions and ensuring that mitigation measures are cost-effective and directed at the most serious problems.

1.4 Weight-of-Evidence Approach

Traditionally, environmental assessments of chemicals have relied on the results of a few relatively simple laboratory bioassays and measured or estimated concentrations in a single medium to predict effects in complex, poorly understood ecosystems (Suter and Loar 1992; Chapman 1995). This approach is fraught with assumptions and uncertainties. Alternative approaches, such as using batteries of tests, field observations, ecoepidemiology, and population and ecosystem modelling, can be used to estimate risk, but each has its own assumptions and associated uncertainties. Rather than relying on a single approach, assessors must evaluate each separate line of evidence, organize these in a coherent fashion, and then use a weight-of-evidence approach to estimate risk (Suter 1993a).

The following should be considered in evaluating each line of evidence (adapted from U.S. EPA 1992):

- *Relevance of the evidence to the exposure scenario of interest.* Lines of evidence that are most relevant to exposure scenarios in Canada are given the greatest weight.
- *Relevance of the evidence to the assessment endpoint.* Toxicity tests that closely mimic field conditions and yield results that are directly related to ecologically significant parameters are given more weight than tests that are less pertinent to field conditions and environmental effects.
- *Confidence in the evidence or risk estimate.* Confidence is a function of the sufficiency and quality of the data and estimation techniques, including adherence to protocols, appropriate experimental designs and associated estimates of statistical power, and theoretical plausibility.
- *Likelihood of causality.* Some lines of evidence, such as observed field effects, may include a variety of stressors in addition to the priority substance of interest. Fox (1991) lists seven principles that can guide assessors in assessing the relationship between a priority substance and an observed adverse environmental effect: time order, strength of association, specificity of association, consistency of the association, coherence of the association, probability, and predictive performance (see Chapter 6 for more details).

By using a weight-of-evidence approach, risk assessment can reduce, but not eliminate, the biases and uncertainties associated with using only one approach to estimate risk. A weight-of-evidence approach is also a useful tool for identifying areas where research is most needed.

1.5 Framework for Ecological Risk Assessment of Priority Substances

The framework for ecological risk assessment of priority substances uses a modification of the one developed by the United States Environmental Protection Agency (U.S. EPA). It incorporates the characterization of entry, exposure and effects that is required to determine whether a substance is "toxic" as defined under Section 11 of CEPA. This framework involves three major steps: problem formulation, analysis, and risk characterization (Figure 1.1; see also U.S. EPA 1992). To ensure that assessments proceed only to the level of refinement required for effective decision-making, a tiered approach has been adopted. Tiers 1 and 2 use, respectively, hyperconservative and conservative point estimates of exposure and effects to determine whether or not a substance has the potential to cause harm in the environment. Tier 3, which is most realistic, compares exposure and effects distributions, rather than point estimates. A special analysis is used for naturally occurring substances. The tiered approach is discussed in detail in Chapter 7. Environmental assessments of priority substances use ecological risk assessment techniques and tools whenever possible and appropriate, particularly in Tier 3 analyses.

Problem formulation focuses on scoping and planning (Chapter 3). Pathways analysis and the identification of sensitive receptors are used to select assessment endpoints (Suter 1993b). As direct toxicity information is not always available for assessment endpoints, measurement endpoints are used to estimate effects on assessment endpoints (Suter 1993b). A conceptual model is then prepared that describes the substance's entry and fate in the environment and its possible environmental effects (Chapter 3). Data gaps that must be filled in order for the environmental assessment to be completed are identified during problem formulation. The PSL framework involves risk assessors, risk managers, and other interested parties during the risk assessment, particularly in the problem formulation stage (see also Hope 1995; Moore and Biddinger 1995). Involving risk managers in the risk assessment process helps to ensure that there is sufficient information to develop appropriate management strategies for substances found to be CEPA "toxic". The involvement of interested parties such as those from other government departments, industry, nongovernmental groups and academia helps to ensure that a broad range of viewpoints is considered.

The analysis phase consists of three major parts: entry, exposure, and effects characterization. The objective of entry characterization is to identify the natural and anthropogenic sources of the substance and to determine the amounts entering the Canadian environment from the various sources (Chapter 4). Entry characterization includes all phases of the life cycle of the substance. Information gathered from the characterization of entry may be used to further refine the problem formulation, as input to the characterization of exposure, and in the development of strategic options during risk management.

The objective of exposure characterization is to determine the estimated exposure value (EEV) or the exposure distribution for each assessment endpoint (Chapter 5). Information must be critically evaluated for quality assurance and quality control (QA/QC). For a Tier 1 hyperconservative analysis, the EEV is usually the maximum measured or estimated concentration in Canada. For Tier 2, it may be possible to reduce the hyperconservative EEV — for example, because bioavailability is expected to be limited — to obtain a more realistic point estimate of maximal exposure. Tier 3 analysis considers the distribution of exposure values, rather than a point estimate, for each assessment endpoint. For wildlife, exposure is usually expressed as a total daily intake or, less often, as an environmental concentration or tissue residue. For quantitative uncertainty analysis using, for example, Monte Carlo simulation, it is necessary to define the distribution for each exposure parameter (e.g., octanol–water partition coefficient K_{ow} ± 95% confidence limits) used in the simulation. For Tier 2 and 3 analyses for naturally occurring substances, natural background concentrations should be estimated as precisely as possible for each area of concern.

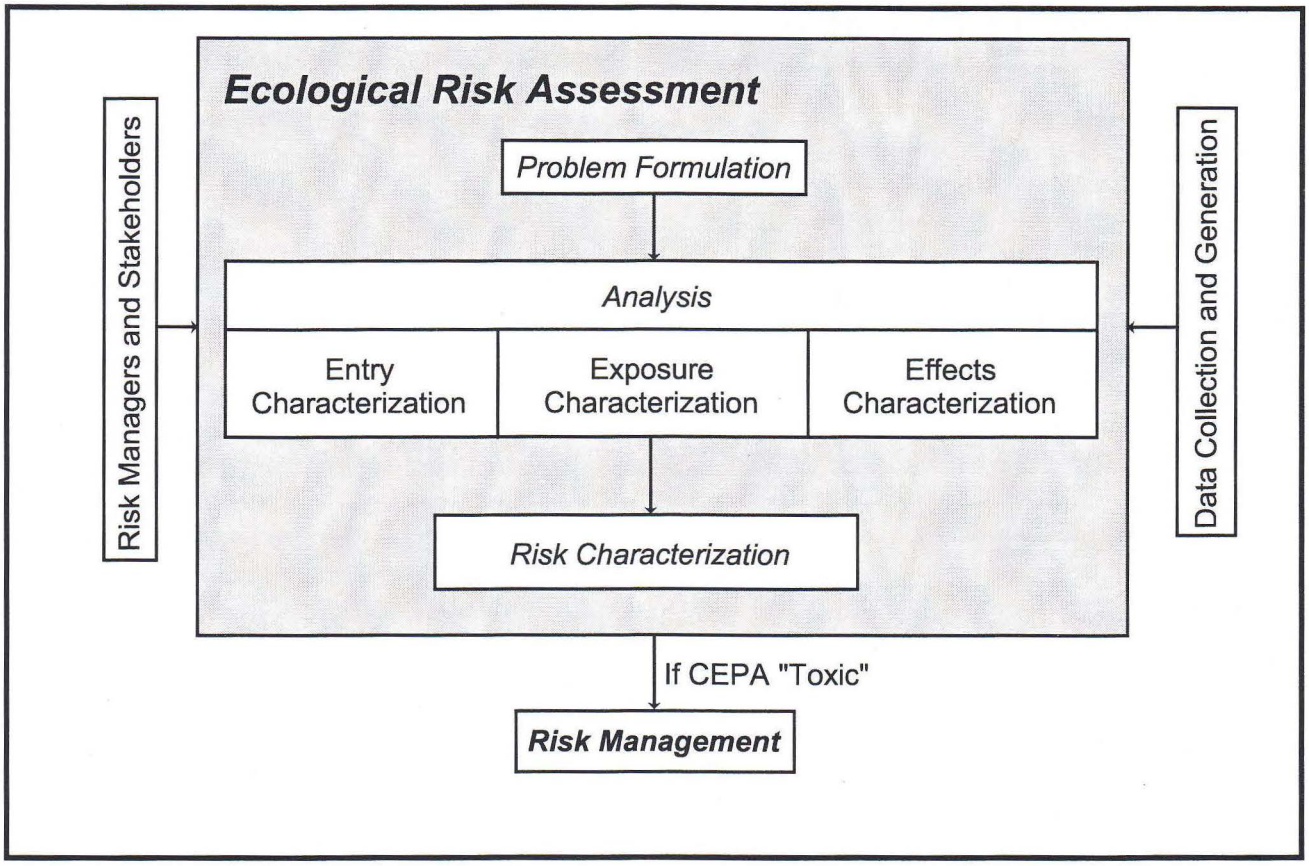

Figure 1.1 Framework for ecological risk assessment of priority substances (modified from U.S. EPA, 1992)

The objective of effects characterization is to determine the critical toxicity value (CTV) or the effects distribution for each assessment endpoint using results of toxicity tests or other studies (Chapter 6). Studies on single- or multispecies toxicity tests, field studies, or critical body burdens (CBBs) can all be used to determine effects. Quantitative structure–activity relationships (QSARs) and equilibrium partitioning (EqP) can be used to corroborate results of toxicity tests or field studies. Toxicity information must be critically evaluated with regard to accepted practices or protocols for QA/QC. The results of toxicity studies on the most sensitive measurement endpoint are used to derive the CTV. In decreasing order of preference, the CTV may be in the form of:

- an IC_{25} (or lower, if the estimate is the result of interpolation) calculated from the concentration–response curve from a chronic or sublethal toxicity test,
- a lowest-observed-effects level (LOEL) from a chronic or sublethal toxicity test,
- a no-observed-effects level (NOEL) from a chronic or sublethal toxicity test, if the LOEL indicates severe effects (e.g., >40% mortality), and
- a median effects concentration (e.g., LC_{50} or EC_{50}) from an acute toxicity test, if chronic or sublethal toxicity data are not available.

Tier 1 analysis uses the CTV for the most sensitive species tested. Tier 2 refines the point estimate by considering, for example, only test results for sensitive species that are most relevant to the assessment endpoints. Tier 3 considers effects distributions, rather than point estimates. For quantitative uncertainty analysis using, for example, Monte Carlo simulation, it is necessary

to define the distribution of each effects parameter (e.g., $IC_{25} \pm 95\%$ confidence limits) used in the simulation.

Risk characterization, the third step in ecological risk assessment, uses a tiered approach. Tier 1 involves dividing the EEV by the estimated no-effects value (ENEV) for each assessment endpoint. For Tier 1, the EEV is generally the maximum measured or estimated concentration in the Canadian environment, whereas the ENEV is calculated by dividing the CTV by an application factor to derive a value with a very low probability of causing adverse effects on the assessment endpoint. If the quotient is <1, the substance is not considered to be "toxic" as defined in Section 11 of CEPA, based on the assessment of that endpoint. If the quotient is ≥ 1 for an assessment endpoint, the assessment should move to Tier 2. Tier 2 involves a further analysis of exposure and effects (see discussion above) to calculate a quotient that is still conservative but more "realistic" than the hyperconservative quotient calculated in Tier 1. If this quotient is <1, the substance is not considered to be "toxic" based on that assessment endpoint. If the quotient is ≥ 1 for an assessment endpoint, the assessment should move to Tier 3. Tier 3 involves comparison of exposure and effects distributions to determine the likelihood of adverse effects in the environment. This approach facilitates a more explicit consideration of sources of variability and uncertainty in the risk analysis. A special analysis is required for naturally occurring substances that have the potential to cause harmful effects, as determined by the Tier 1 analysis. This analysis requires adjusting the effects characterization to take into account the tolerance of organisms normally found in naturally enriched areas. If the analysis indicates that anthropogenic sources can cause harmful effects to organisms normally found in areas of interest, then the substance is declared "toxic". A detailed discussion of the tiered approach is presented in Chapter 7.

In some assessments, it may be possible to estimate the ecological consequences of exposure to a substance through the use of field studies, population models, or food web models. This information can be helpful to risk managers to identify the various actions that could be taken to protect the environment.

Complex substances such as mixtures and effluents are on the second PSL. The interactions of individual constituents in a complex substance can cause a harmful effect that is qualitatively or quantitatively different from that of the constituents acting alone. Effects of two or more interacting substances may be additive, antagonistic (i.e., less than additive), or synergistic (i.e., more than additive). Therefore, complex substances require different methods for assessing environmental risks. Chapter 8 discusses such methods. The chapter focuses on the differences between assessments of complex and individual substances, with particular emphasis on effects and risk characterization.

This guidance manual presents a number of approaches and tools that can be used in environmental assessments of priority substances. Assessors, in consultation with risk managers, must decide which approaches and tools to use for their particular assessments. In general, existing data should be used whenever possible. Uncertainty and variability must be identified, quantitatively whenever possible, and their effects on the assessment discussed. Assessors must determine if further data are required to complete the assessment and arrange to have research carried out to generate these data. Because of the expense and time required for toxicological tests and environmental monitoring, additional data should be generated only when uncertainties around an assessment are unacceptable and hence do not allow for a conclusion concerning CEPA toxicity to be made. Assessors should reevaluate data requirements and availability as they begin each successive tier of the assessments.

1.6 Some Points to Remember

- Explicitly state the scope and objectives of the assessment.
- Set out the content impartially, with a well-balanced treatment of the evidence bearing on the conclusions.
- Convey uncertainty explicitly and fairly. State and justify all assumptions. Where possible, include a discussion of the research that might decrease the degree of uncertainty.

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CHAPTER 2
DATA COLLECTION AND GENERATION

2.1 Introduction

This chapter provides an effective approach to collect and generate data required for environmental assessments of priority substances under CEPA. Chapter 2 of the resource document provides details about information sources available to collect and generate these data, with emphasis on data collection.

Data used when conducting assessments of priority substances must be of acceptable quality. All key data must be verified by consulting their primary source. Assessors should obtain original references to critically and scientifically evaluate the data. In cases where sources of information are incomplete (e.g., information on detection limits, sample sizes, measured concentrations, etc. is not reported), assessors should contact individual authors to obtain the data necessary to evaluate the study. Also, erroneous data may result from transcription or typographical errors during the process of publication or database development. As both published and unpublished data vary in quality, assessors should become familiar with issues of data quality. Specific QA/QC issues are addressed where applicable throughout this manual and the accompanying resource document.

The data collection and generation process described below has been designed as a flexible guideline for assessors. While this process is an effective approach for obtaining most types of data required for assessments of priority substances, information gathering may need to be customized on a substance-by-substance basis. The lead assessors, with input from their environmental resource groups, will make decisions regarding the quantity and quality of data for the assessment. As with the problem formulation phase of an assessment, data collection is an iterative process, and many of the following steps may need to be revisited throughout the assessment process as additional keywords, data sources, or data needs are found. Guidance on search strategies is provided in the chapter.

2.2 Stage One: Data Gathering Required for Problem Formulation

The first stage of the data collection and generation process involves gathering data required for problem formulation, from initial scoping through to the development of a conceptual model (Chapter 3). The aim of the first stage is to complete a thorough review of existing sources of information about the substance and to identify as early as possible any data gaps.

At an early stage in the data collection process, assessors should develop a set of keywords that will be used to search for information in databases. The chemical name, Chemical Abstracts Service (CAS) number, and synonyms are a good starting point for single chemicals. Keywords should be refined when necessary during the data collection process to obtain all available data. Assessors should always obtain references for important data cited in journal articles, reports, and databases. These references can verify that data had been correctly cited and may also lead assessors to new sources of information. Additional guidance on search

strategies for mixtures and effluents is presented in Chapter 8. Data gathered during stage one are then used to develop an initial conceptual model for the assessment.

2.2.1 Data Provided by the Priority Substances List (PSL) Secretariat

Scientific dossiers prepared by the PSL Secretariat are made available to assessors. These dossiers include basic information about the substance's chemical identity and physical and chemical properties. They also provide an initial review of toxicological and entry data, international assessments, and the rationale provided to the Ministers' Expert Advisory Panel to recommend the substance for the PSL. For many substances, the information provided by the PSL Secretariat may be sufficient to complete the initial scoping stage of the assessment. These data may not be sufficient to conduct initial scoping of complex substances; thus, more extensive data collection may be required (consult Chapter 8 on mixtures and effluents for additional guidance).

2.2.2 Existing International Assessments

The objective of this step is to collect and review relevant ecological assessments that have been conducted by organizations such as the U.S. EPA or the Chemicals Program of the Organisation for Economic Co-operation and Development (OECD). These assessments may provide valuable scientific data and references. They may also provide assessors with an overall picture of the key issues in the assessment.

2.2.3 Desk References

Desk references can provide valuable environmental information. Sources that should be consulted include chemical dictionaries, encyclopedias, guideline reports, handbooks of physicochemical properties, texts summarizing environmental fate and exposure data, etc.

2.2.4 Readily Available Databases/ Catalogues

After reviewing PSL dossiers, international assessments, and desk references, assessors should conduct an extensive literature review with a focus on Canadian data. Assessors should begin with the variety of information sources available at low cost, including Environment Canada information holdings and databases. This first general search for data should be conducted with the keywords identified previously.

2.2.5 Commercial Databases

Assessors should review the data gathered thus far. Once data gaps are identified, keywords should be redefined and the search criteria tailored to target missing data. Assessors should use the information presented in Chapter 2 of the resource document to select commercial databases with the appropriate focus and scope for the types of data required. The search strategy for a particular substance may need to be changed depending on the focus of a given database. The retrieval of irrelevant or duplicate data can thus be minimized.

2.2.6 Specialty Resources

In order to ensure that all existing data have been found to fill data gaps, assessors should conduct a careful search of specialized inventories, databases, or reports. Assessors should use their knowledge of the substance to identify individuals or groups that likely have specialized published or unpublished data. Industry associations, other federal government departments, and provincial/ territorial governments will be important resources in this process.

2.2.7 Concluding Stage One

The data collected are then reviewed, focusing on the most relevant publications and reviews to build an initial conceptual model that can be discussed with interested parties and refined throughout the assessment. While additional data are being collected during stages two, three, and four, assessors should critically review the data used to develop their initial conceptual model to confirm that these data are valid.

2.3 Stage Two: Problem Formulation Refinement with Participation of Interested Parties

In stage two, environmental resource groups and interested parties are invited to help refine the problem formulation. As well, assessors identify

people and groups whose information or expertise could assist with the assessment.

2.3.1 Consultation with Interested Parties

Assessors should consult with risk managers, Environment Canada regional offices, research institutes and other interested parties including other government departments, provinces and territories, industry associations and representatives, environmental groups, and academia. Such consultations provide an opportunity to tap into scientific and technical support and expertise. They also provide an effective approach to quickly obtain unpublished data. This step also provides a forum to develop partnerships required for research.

2.4 Stage Three: CEPA Section 16 and Section 18 Notices

Sections 16 and 18 of CEPA may be used to obtain information from Canadian manufacturers, importers, and users of PSL substances on a compulsory basis. This approach allows for a consistency and completeness in data gathering.

Section 16 of CEPA authorizes the Minister of the Environment to gather existing data for the *purpose of assessing whether a substance is toxic or capable of becoming toxic*. Assessors can determine whether the required data exist, so that data gaps critical to the assessment can be identified and filled.

Section 18 of CEPA can be used when the Ministers of Environment and Health have *reason to suspect that a substance is toxic or capable of becoming toxic*. Section 18 provides three methods to gather data about a specified substance. A notice may require that those involved with the substance notify the Minister of the Environment of their involvement, provide specified information in their possession or to which they can reasonably be expected to have access, or perform toxicological and other tests specified by the Minister and submit the test results once completed.

Data gaps should be identified as early as possible in the problem formulation phase, as preparing and executing notices may take several months. The Use Patterns Section of the Chemicals Control Division of Environment Canada will work in conjunction with assessors to prepare Section 16 and Section 18 notices. Before notices are sent out, assessors should identify the appropriate industry sectors or companies to which they should be sent and clearly define the types of information required. This ensures that notices are read and acted upon by people knowledgeable in the area and that replies will be useful to the assessment.

2.5 Stage Four: Generation of Data Through Research

Research activities will be coordinated from a program perspective by the Chemicals Evaluation Division of Environment Canada to ensure a consistent approach and efficient and cost-effective use of resources.

2.5.1 Recommendation of Research Activities

As part of problem formulation, assessors should identify any research activities that are essential for reaching a conclusion about whether or not their substances are CEPA "toxic". An ecological risk assessment review group will review the proposed data generation needs and identify overall priorities and the most efficient means of fulfilling those needs. The lead assessors will be responsible for overseeing the generation of data for their substances. Appropriate partners should be involved in the conduct or sponsorship of this work.

CHAPTER 3

PROBLEM FORMULATION

3.1 Introduction

3.1.1 Goals and Objectives

Problem formulation is the planning phase in the ecological risk assessment framework. Here, the goals and focus of the assessment are established, data gaps are identified, and a strategy for proceeding with the assessment is devised. This phase includes the development of an *initial scoping* and a *pathways analysis*, consideration of *receptor sensitivity*, analysis of the *ecological relevance* of potential receptors, selection of *assessment endpoints* and associated *measurement endpoints*, and the development of a *conceptual model* (Figure 3.1).

In the problem formulation phase, risk assessors begin working with risk managers in Environment Canada and with interested parties in other governmental departments, industry, non-governmental organizations and academia to ensure that the environmental assessment will have a firm scientific basis and will ultimately be useful for decision-making.

An example of a problem formulation is presented in Section 3.3 of the resource document.

3.1.2 Relationship with Other Phases

Information set out in the problem formulation phase is used as the starting point for more in-depth analyses that follow during the characterization of entry, exposure, and effects. It is thus important that an initial problem formulation be completed as early as possible in the assessment process. Problem formulation is an iterative process. When little information about a substance is available at the beginning of the process, the initial problem formulation will be general and qualitative. As more information is obtained and analyzed, the problem formulation will become more focused, become more explicit in its identification of assessment and measurement endpoints, and present more quantitative details. As the environmental assessment proceeds through the entry, exposure, and effects characterization phases, problem formulation should be updated to serve as a running summary of the assessment.

3.2 Initial Scoping

Initial scoping begins by considering the rationale that the Ministers' Expert Advisory Panel on the Second Priority Substances List (Ministers' Expert Advisory Panel 1995) gave for selecting the substance and the expected focus of the assessment. Additional preliminary information is gathered at this stage (see Section 2.2).

Information about the identity of the substance is presented in the initial scoping stage, including an internationally accepted chemical name, following rules established by the International Union of Pure and Applied Chemistry (IUPAC) or the CAS, other commonly used synonyms and trade names, and the CAS Registry Number, when available. For elements, the relative abundances of isotopes, oxidation states in the environment, and the identities of common environmental forms should also be determined. This information is needed to permit an efficient literature search and other data-gathering activities. In addition, the molecular structure of organic chemicals should be elucidated for possible use in models or QSARs for exposure or effects characterization (Chapters 5 and 6).

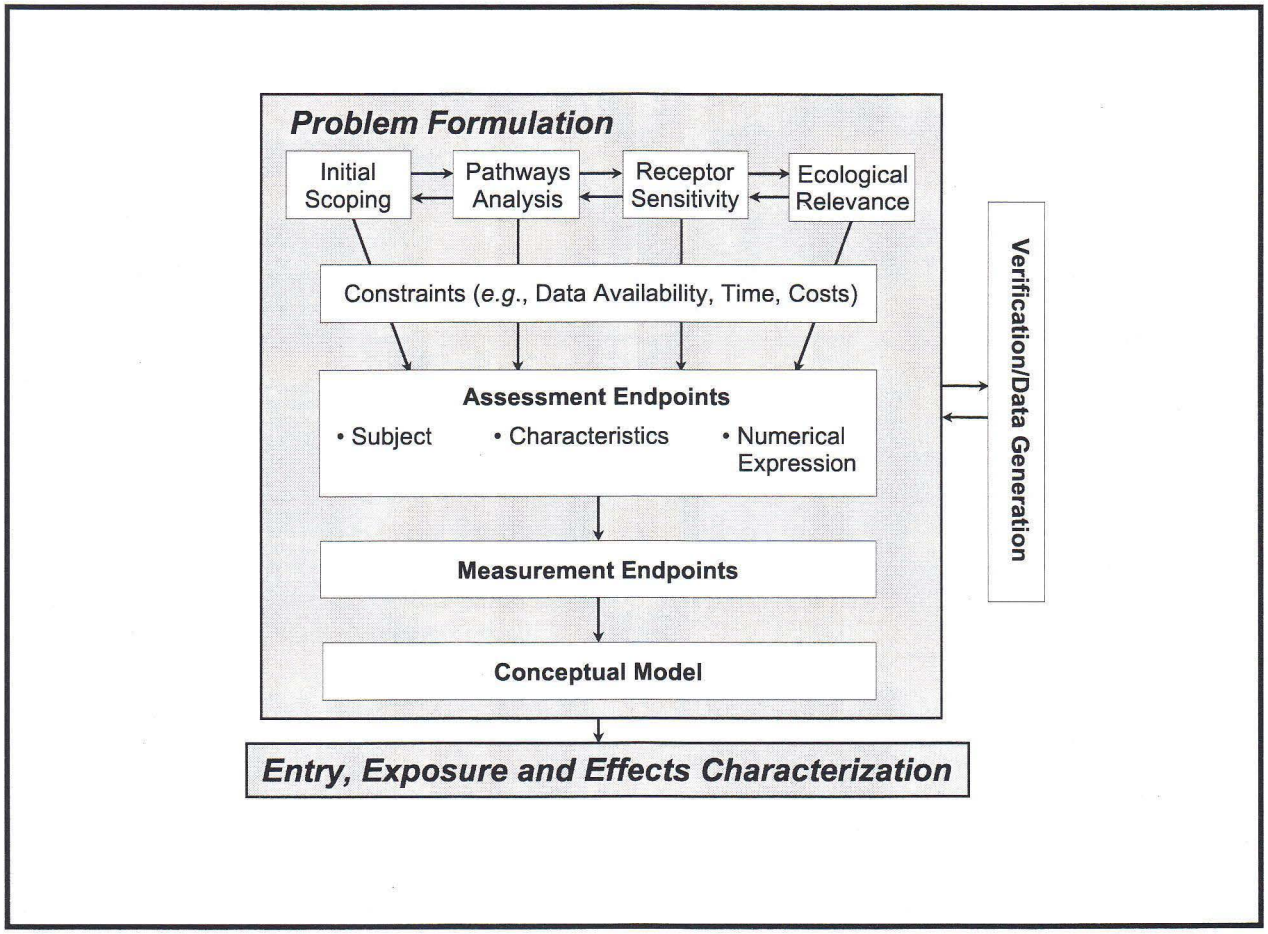

Figure 3.1 The problem formulation phase in the ecological risk assessment framework for priority substances

Physical and chemical properties of the substance should be determined for predicting its environmental fate and potential effects. For organic substances, these usually include molecular weight, molecular volume, water solubility, vapour pressure, partition coefficients, and dissociation constants. For inorganic substances, relevant properties vary depending upon the chemical forms (e.g., atoms, compounds, or complexes). Important parameters for inorganic substances include atomic or molecular weight, water solubility, equilibrium constants, and vapour pressure. Values chosen for key parameters used in fate or exposure models may significantly affect model predictions. Therefore, values for key parameters should be determined as accurately as possible and any uncertainty clearly presented. Experimental methods of quantification are preferred, but calculated values based on QSARs, for example, may be acceptable at this stage.

3.3 Pathways Analysis

Pathways analysis considers a substance's entry into the environment and its probable environmental fate. This analysis is used to predict a substance's geographic distribution and fate in the Canadian environment and to identify potential receptors that may be exposed to it.

Consideration must be given to the potential for environmental releases at any stage of a commercial substance's life cycle, from manufacture through distribution and use to final disposal. A substance may also enter the Canadian environment in other ways — for example, from natural sources, by transboundary transport, as a transformation product of another substance, or as a component of a mixture.

To characterize environmental releases, information is required on:

- amounts manufactured, imported, and exported,
- specific uses, including amounts used for various applications,
- significant sites of release in Canada from human activities and from natural processes,
- amounts, forms, and conditions under which the substance is released into the Canadian environment,
- temporal patterns of releases (e.g., continuous, intermittent, seasonal), and
- environmental compartments (e.g., air, water, soil) receiving releases.

This information enables assessors to estimate how much of the substance is being released into the Canadian environment and where and how often these releases are occurring. This information also serves as a starting point for the next step — characterization of the substance's environmental fate.

A substance's environmental fate may be characterized by:

- identifying its probable environmental partitioning to air, soil, surface water, groundwater, sediment, and biota and estimating its persistence in these compartments,
- estimating its geographic distribution and concentration ranges in the Canadian environment,
- identifying ecosystems that may be exposed to the substance, and
- identifying living or nonliving components of the ecosystems that may be exposed.

Information about a substance's physical and chemical properties, amounts released into various compartments of the environment and persistence in these compartments, the identity of its transformation products,[1] and its bioavailability and tendency to bioaccumulate in living tissue may be required for models that can help to characterize the environmental fate of a substance and to define sensitive parameters and data gaps when establishing research priorities. The characterization of the environmental fate of a substance is discussed in more detail in Section 5.3.

Information about quantities of a substance released in specific regions within Canada can be used to predict its concentration in various environmental compartments in these regions. Models may be used to make such predictions (see Chapter 5). If Canadian environmental monitoring data are not available, data from similar areas, such as the northern United States, may be used to support the plausibility of predicted environmental concentrations. A discussion of the characterization of environmental concentrations is presented in Section 5.6 of the resource document.

From the initial characterization of environmental partitioning and fate and predicted environmental concentrations, it is possible to predict, in a general way, ecosystems that are at risk (e.g., aquatic ecosystems). When specific sites of release are known, it is then possible to identify the ecosystems more precisely (e.g., a specific stretch of a river). Within ecosystems, particular components may be exposed to the substance under investigation. For example, benthic organisms are likely to be exposed to substances that partition to sediments. When precise ecosystems have been identified, it is then possible to more precisely identify the components of those ecosystems that may be exposed (e.g., benthic organisms in a specific stretch of a river).

Nonliving components of the environment upon which human life depends may also be exposed and considered in the environmental assessment. For example, stratospheric ozone may be exposed to persistent substances that reach the stratosphere when released into air.

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[1] A transformation product may itself have the potential to cause adverse effects in the environment. If such a product is present in the environment primarily because of the transformation of the parent substance, the potential risks of the transformation product could be assessed along with those of the parent. If there are other major sources of the transformation product, the product should be considered as a candidate for a separate assessment (see further discussion in Section 5.4 of this guidance manual and the resource document).

3.4 Receptor Sensitivity

Consideration of receptor sensitivity involves the analysis of information about the substance's mechanism of toxicity and effects data from laboratory or field studies. This information is used to identify species or larger taxonomic groups that are particularly sensitive to the substance and to determine concentrations or doses that cause adverse effects. QSARs may also be used in the initial identification of sensitive organisms. Often, the identity of particularly sensitive organisms is unknown. It is therefore desirable to review effects data from a battery of toxicity tests using organisms from several taxonomic and trophic levels. Such organisms should be representative of biota in the environmental compartment(s) to which the substance of concern is believed to partition.

3.5 Ecological Relevance

The environmental roles of highly exposed or sensitive receptors should be analyzed in order to identify the receptors' ecological relevance and to predict possible indirect effects on other ecosystem components, such as predator or prey species. This can be accomplished by considering the receptors' life cycles and by determining any special functions that they may have in the environment. For example, microorganisms may be vitally important in nutrient cycling, and earthworms are important for the aeration and conditioning of soil.

The results of the initial scoping exercise, pathways analysis, and consideration of receptor sensitivity and ecological relevance are then used to select assessment and measurement endpoints.

3.6 Choosing Assessment Endpoints

An assessment endpoint is "a quantitative or quantifiable expression of the environmental value considered to be at risk in a risk assessment" (Suter 1993). Potential assessment endpoints exist for all ecological levels of organization (U.S. EPA 1992a; ASTM 1994). Possible assessment endpoints at the ecosystem level include primary productivity, energy flow, nutrient cycling, and decomposition of organic matter. At the community level, assessment endpoints could include biodiversity, including species richness and evenness, and food web structure. Possible assessment endpoints at the population[2] level could include population abundance, reproductive success, and age and size structure. At the individual level, assessment endpoints could include survival or physiological status, reproductive capacity, growth rate and development, and behaviour. When expressing an assessment endpoint, assessors should identify an ecological component, such as a trout population, and a characteristic of that component, such as reproductive success.

Assessment endpoints selected at the population level will probably be most common in PSL assessments. In many cases, abundance of the most sensitive species in each environmental compartment of concern may be a practical assessment endpoint to consider first. Consideration of the species' role in the environment may suggest that an assessment endpoint at a higher level in the ecological hierarchy (i.e., ecosystem > community > population) may be more appropriate. For example, an adverse effect on microorganisms that are important decomposers may indicate an ecosystem endpoint such as "the rate of nutrient cycling." When it is not possible to select assessment endpoints above the population level, it may still be useful to indicate potential direct or indirect effects at higher levels, recognizing that extrapolating up the ecological hierarchy introduces additional uncertainty at each step.

Several assessment endpoints are needed to assess substances that partition to more than one environmental compartment or that occur in the environment in a number of geographic areas. Furthermore, selection of several assessment endpoints ensures that a range of ecosystem components is considered in the assessment.

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[2] A "population" may be defined as a collective group of organisms of the same species occupying a particular space and having the potential to reproduce.

3.7 Choosing Measurement Endpoints

A measurement endpoint is "a quantitative summary of the results of a toxicity test, a biological monitoring study, or other activity intended to reveal the effects of a substance" (Suter 1993). Each assessment endpoint must have one or more measurement endpoints. Measurement endpoints are needed because assessment endpoints often refer to characteristics of populations, communities, and ecosystems defined over fairly large geographic areas and relatively long time periods. These factors make the direct measurement of effects difficult or impossible. The relationships between assessment and measurement endpoints must be clearly described.

Unlike assessment endpoints, measurement endpoints are commonly selected at the individual level of the ecological hierarchy. If an assessment endpoint is the population abundance of a particular species of fish, an appropriate measurement endpoint could be the result of an acute or chronic toxicity test using the same species or a related species. Similarly, if abundance of an endangered raptor were chosen as an assessment endpoint, dietary LD_{50} values from studies with another bird species would be an appropriate measurement endpoint. For the protection of terrestrial plants, necrosis, chlorosis, or reduction in growth of legumes or conifer seedlings resulting from soil or atmospheric exposure to the substance could be used as the measurement endpoint.

Acceptable measurement endpoints for ecosystem-level assessment endpoints include measurements of total biomass, productivity, and nutrient dynamics derived from microcosm or mesocosm studies or from field surveys if a cause-and-effect relationship can be established. Acceptable measurement endpoints for community-level assessment endpoints include number of species, measures of species evenness, community quality indices, and changes in community type derived from microcosm studies or field surveys. Acceptable measurement endpoints for population-level assessment endpoints include abundance, age and size distributions, reproductive performance, and frequency of mass mortality derived from toxicity test results or field surveys (ASTM 1994). Lethality and reproductive impairment, measured in laboratory toxicity studies, provide a strong link to the potential effects of the substance on the growth and survival of natural populations.

3.8 The Conceptual Model

A conceptual model describes as explicitly as possible a substance's predicted fate, the mechanisms by which it could affect assessment endpoints, and the likely ecological consequences of these effects. The level of detail, the information needed, and the methods to be used to complete the assessment, including any research needed to fill data gaps, should also be specified.

The conceptual model is developed by constructing a series of qualitative exposure scenarios that describe how the priority substance could affect the assessment endpoints. Each scenario defines the assessment and measurement endpoints, their relationship, and spatial, geographic, and temporal scales (U.S. EPA 1992b). Each scenario should also describe the methods and analyses that will be used to estimate risk. As there is no universal method for quantifying environmental risk, several methods that aid in the process should be specified (Suter and Barnthouse 1993). Possible methods include:

- field studies or fate models to estimate exposure,
- statistical regression techniques to estimate effects levels for measurement endpoints,
- the quotient method to compare exposure and effects estimates,
- use of empirical field data or Monte Carlo analyses to estimate the probabilities of specified effects, and
- population models to estimate, for example, risks of extinction over a given time period.

The rationale for choosing a particular scenario or method should be documented (U.S. EPA 1992b).

Assessors should consult with risk managers at Environment Canada (e.g., Commercial

Chemicals Evaluation Branch, National Office of Pollution Prevention, or Air Pollution Prevention Directorate, depending on the type of substance) to determine if the proposed conceptual model will provide information to support any subsequent risk management decisions. Assessors should also discuss the conceptual model with interested parties and selected experts to refine the proposed model and to prepare plans to conduct new studies if necessary. When the conceptual model and the plan to carry out the assessment have been determined, the detailed entry, exposure, and effects characterization phases of the environmental assessment can begin.

An example of a conceptual model is included in Section 3.3 of the resource document.

3.9 Some Points to Remember

- Consult other interested parties and involve them in the scoping process.
- Identify and involve experts in the assessment. Assessors often feel that opening up the process leads to additional out-of-scope requirements and could adversely influence the scientific integrity of the assessment. Although such concerns are sometimes warranted, the risk assessment is far more likely to lead to effective risk management decisions if assessors and interested parties have a clear understanding of the assessment objectives and methods at the outset (Hope 1995).
- Present and review all relevant information.
- Present the rationale for choosing assessment and measurement endpoints.
- Present the conceptual model used for risk analysis and risk characterization.

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CHAPTER 4

ENTRY CHARACTERIZATION

4.1 Introduction

4.1.1 Goals and Objectives

The entry characterization phase identifies the anthropogenic and natural sources of a substance and estimates the amounts and frequencies of its release into the Canadian environment. This information is then used to assess the relative significance of various sources and help define the spatial and temporal scales for the assessment.

4.1.2 Relationship with Other Phases

In the entry characterization phase, the entry portion of the pathways analysis developed during problem formulation is verified and refined. This is achieved by accurately identifying and quantifying the various sources and releases. Entry characterization sets the stage for the characterization of exposure. For example, information about sources and releases is required as inputs to fate and transport models (Chapter 5). For substances declared "toxic" as defined in Section 11 of CEPA, entry characterization provides information essential for developing strategic options.

Access to current and accurate information is key to completing an accurate and useful risk assessment. Chapter 2 describes several mechanisms by which to obtain entry information. This information is often difficult to obtain because it is typically site-specific and is usually not available in the published literature. To overcome these difficulties, it is imperative to establish, as early as possible, a forum for the efficient exchange of information among risk assessors, risk managers, and other interested parties.

Figure 4.1 summarizes the main steps involved in entry characterization.

4.2 Identification of Sources

The first step in entry characterization is to identify a substance's sources in Canada. This includes natural and anthropogenic sources and transboundary sources. Although major sources should have been identified during the problem formulation stage, some significant sources may have been missed, or data may have been lacking.

4.2.1 Natural Sources

Inorganic and organic substances may be produced by a wide variety of natural processes. All processes leading to a substance's release into the Canadian environment should be identified so that effects due to anthropogenic versus natural sources can be differentiated.

Natural sources of inorganic substances to the atmosphere include windblown dusts, sea spray, volcanic emissions, crustal degassing (Rasmussen 1994), volatile exudates from plants, volatile compounds formed by soil microbial activity (Cullen and Reimer 1989), and natural combustion events (Havas and Hutchinson 1983). For soil, bedrock or glacial deposits from which it was derived are the primary natural sources. Inputs also occur from natural atmospheric fallout and from sediment deposits in areas subjected to periodic flooding. Primary natural sources of inputs to aquatic systems are weathering and erosion of geological materials and natural atmospheric fallout.

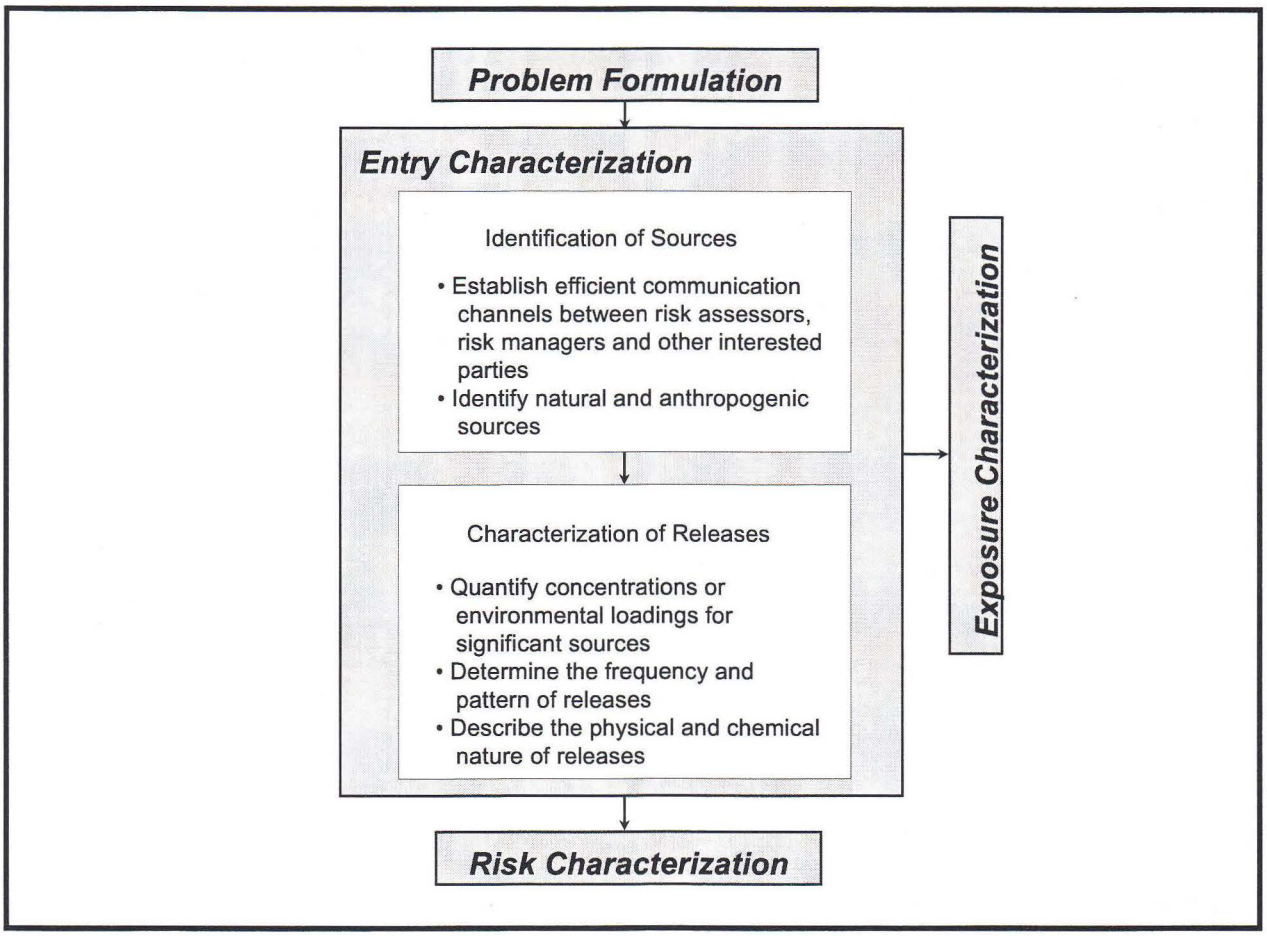

Figure 4.1 Entry characterization in the ecological risk assessment framework for priority substances

Many organic substances, including halogen-containing chemicals, may be produced by natural processes. Many types of organisms, including terrestrial plants, fungi, microorganisms, and mammals, contain haloperoxidase enzymes that can halogenate organic compounds in the presence of chloride, bromide, or iodide (Gribble 1994).

4.2.2 Anthropogenic Sources

Environmental releases can occur at any time during a substance's life cycle, including production, transportation, use, and disposal.

Manufacturing sites, which may include raw material extraction and chemical syntheses, should be identified along with estimates of annual production at each site. Releases at the manufacturing and processing stage may take a variety of forms, including liquid effluents, stack gases, and accidental or fugitive emissions.

The amount of the substance imported annually into Canada should be determined, along with its destination by province/territory or city.

Expected modes of transportation, distribution, and storage should be identified, because environmental releases can result from accidents such as pipeline ruptures, train derailments, tank truck collisions, and leakage from storage tanks.

The specific uses and applications of the substance in Canada should be determined. When possible, this should include the identity and locations of industrial, commercial, and institutional users of the substance. Information about the substance's domestic or household uses should also be obtained.

Required information about the disposal of the substance includes disposal sites and a general description of disposal methods. Different environmental compartments may be affected,

depending upon the treatment or disposal method employed. For example, incineration can result in significant atmospheric emissions as a result of incomplete combustion or reactions of components in stack gases. Landfills that are not adequately sealed can release soluble substances to local soils and groundwater. Disposal of municipal sewage sludge on agricultural land can result in releases of volatile substances to air and soluble substances to local soils and groundwater (Webber and Shamess 1987; Webber 1990).

4.2.3 *Transboundary Sources*

Substances can enter the Canadian environment through long- and short-range transport. Transboundary transport is a well-known source of persistent substances, but it can also be significant for less persistent substances if an important source is located near the Canadian border. An example is smog and incinerator emissions migrating from Detroit into the Windsor area. Entry of substances into Canada by aquatic transboundary transport has been well documented. An example is the contamination of the Great Lakes and St. Lawrence River from landfill sites in the United States.

4.2.4 *Indirect Sources*

In addition to the direct releases listed above, some substances can be formed in the environment from other synthetic substances as a result of natural biotic or abiotic transformation processes. Trichlorobenzenes, for example, can be formed in anaerobic sediments by reductive dechlorination of more highly chlorinated benzenes (Hollinger *et al.* 1992). Such processes should be identified and their contribution to measured ambient exposures taken into account.

4.3 Characterization of Releases

Once the key sources have been identified, entry characterization should focus on a more refined analysis of the specific characteristics of the releases. Data gathered during this step should, to the extent possible, be quantitative. The objectives are to:

- quantify the substance's releases in Canada,
- identify the frequency and patterns of the releases, and
- describe the substance's physical and chemical nature.

4.3.1 *Quantifying Releases*

Releases of a substance can be characterized in several ways. Key quantitative parameters are concentrations of the substance in effluents, stacks, or the receiving environment and environmental loadings — amounts released per unit of time.

In general, site-specific monitoring data provide the most accurate means of estimating substance concentrations and rates of release in stack gases, effluents, spills, etc. (Carpenter *et al.* 1990). However, monitoring data are often unavailable. Even when such data exist, their quality can vary depending on the location of sample stations, the accuracy of monitoring techniques, and the timing of sampling and release events. Also, because of the nonpoint nature of many natural sources, it is often difficult to obtain accurate empirical estimates of natural release rates. In cases where monitoring data are of insufficient quality or quantity to allow the reliable quantification of releases from major sources, release estimates may be based on model calculations or emission factors.

Models used to characterize releases may be simple mass-balance types, requiring information on a few easily obtained parameters, or more complex ones, requiring more extensive information on system processes, data from monitoring programs, historical records, or assumptions about probability distributions. Case Study 4.1 in the resource document provides an example of a simple mass-balance model used to quantify releases from municipal wastewater treatment plants. This type of model can also be used to quantify releases from natural sources, if steady-state conditions in the receiving compartment are assumed. Case Study 4.2 in the resource document provides an example of the use of a more complex model.

Emission factors are usually expressed as the mass of a substance emitted per unit of mass or volume of product or per unit of time during a production process. Factors may be generated using monitoring data, models, or professional judgment. Lists of factors for predicting releases of

substances from industrial sources have been compiled by various national and international agencies (e.g., CEU 1995). Care must be used when applying such factors to ensure that they are based on conditions that are relevant to the industrial processes and emissions control technology currently used in Canada. Release estimates based on emission factors are generally less reliable than those based on monitoring or site-specific models. If the uncertainty surrounding the estimates of releases is judged to be unacceptable, it will be necessary to confirm the estimates using empirical data. Case Study 4.3 in the resource document provides an example of how emission factors may be used to estimate releases of an organic chemical associated with different commercial applications.

Release data pertaining to leakage from storage facilities or to accidents during transportation are not always available. These data may be of limited use in estimating exposure, as the magnitude and locations of such releases are often not adequately reported. Material balances showing the volumes of substances being transported, the principal modes of transportation, the physical form of the substance during transport, and the locations of shipping and receiving points may be useful in identifying areas that are most at risk of exposure from some of these inadvertent releases.

4.3.2 Frequency and Patterns of Releases

The frequency and patterns of releases from each major source should be determined whenever possible. For example, a substance may be released from a site continuously or intermittently. The quantities that are released may vary with the seasons. If releases are intermittent, monitoring periods must be long enough to allow the distribution of their severity and the time interval between releases to be ascertained. Seasonal variations in release rates should be determined, as variations can affect loading estimates, which are needed to make meaningful exposure estimates.

The quantity of a substance released into the environment varies depending upon its use. Solvents used for cleaning are highly dispersive; much of the amount used is released into the environment. Chemical intermediates, on the other hand, are usually consumed in chemical processes and are released in only limited quantities. Estimates of the amounts of a substance used in different applications, combined with dispersivity data, can indicate the magnitude of releases in different areas.

When comparing releases from different sources, it is important to recognize that the magnitude and spatial extent of environmental impacts may differ depending on whether releases are point or nonpoint. For example, while the absolute magnitude of releases from nonpoint sources may be large, the environmental impact may be small if releases are spread over wide areas. Conversely, although releases from a point source may be small in absolute terms, they may cause significant harm locally if they are confined within a limited area.

4.3.3 Chemical and Physical Nature of the Substance Released into the Environment

An analysis of a substance's physical and chemical properties should be conducted for each significant source. This is used during exposure characterization to gain an understanding about how a substance is likely to partition in the receiving environment.

Assessors should obtain site-specific information about a substance's physical forms and chemical nature. This is especially important for metals and other chemical elements that can be released in a variety of forms, each with its own reactivity and mobility properties. For organic substances, the chemical form is usually defined, but physical phase association (e.g., aqueous solution or suspended solid in an effluent) can vary. This may be an important fate determinant. For solids released into air and water, properties of particular importance include density, size and shape (which determine their rates of removal by gravitational settling), and solubility (which determines their persistence in the solid form and ultimately their bioavailability) (Webber and Shamess 1987; Webber 1990).

4.3.4 Recognition of Trends in Releases

Changes in release quantities and patterns may occur because of changes in the quantity of a substance produced or used at a facility. They

can also occur as a result of changes in industrial processes or waste treatment technologies. Therefore, it is necessary to note any recent trends in environmental releases, so that possible exposure scenarios may be considered during the exposure characterization phase. For example, it may take many years for a persistent substance to disappear from sediments, soil, or groundwater, even if releases have been stopped or severely reduced. Less persistent chemicals would disappear more quickly. In these cases, assessors may need to obtain sufficient data about past releases so that the relative contribution of recent loadings can be estimated. Any anticipated increases or decreases in releases or changes in release patterns should be noted so that future exposure scenarios may be predicted and taken into account in the assessment.

4.4 Some Points to Remember

- Identify and quantify potential sources, levels in the environment, pathways, and routes of exposure, and acknowledge and estimate uncertainties in these values.

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CHAPTER 5

EXPOSURE CHARACTERIZATION

5.1 Introduction

5.1.1 Goals and Objectives

The purpose of this phase of the assessment is to quantify contact between a substance[1] that has been released from anthropogenic sources and appropriate receptors.[2] The primary outputs are EEVs, expressed as concentrations or doses for identified receptors in areas of concern. Estimates of natural contributions to EEVs may be required for natural substances. Figure 5.1 summarizes the principal steps involved in detailed exposure characterization.

5.1.2 Relationship with Other Phases

Exposure characterization builds upon the pathways analysis portion of initial problem formulation (Chapter 3) and release information obtained from detailed entry characterization (Chapter 4). A calculated or measured maximum EEV is used as the numerator in a risk quotient for Tiers 1 and 2; frequency distributions are used to characterize EEVs for Tier 3 (Chapter 7). Estimates of natural contributions to exposure may be used during risk characterization (Chapter 7), to set lower bounds on ENEVs for natural substances and to evaluate the potential for natural tolerance in receptor organisms.

5.2 Pathways Analysis

Detailed pathways analysis for a substance should integrate data on:

- its releases from identified anthropogenic sources,
- its physical and chemical properties and those of the receiving environment, and
- key transport and transformation processes.

The objective is to refine the initial pathways analysis developed for problem formulation and to verify the environmental media in which the substance accumulates, as well as the size and location of the areas likely to be affected. The identity and main routes of exposure of the principal receptors should also be verified at this stage. A table listing the primary routes of exposure for different classes of organisms is provided in Chapter 5 of the resource document.

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1 Exposure characterization for complex mixtures and effluents is described in Chapter 8.

2 When receptors are wildlife species (birds, mammals, amphibians, or reptiles), assessors should contact the Canadian Wildlife Service of Environment Canada for additional guidance on exposure characterization.

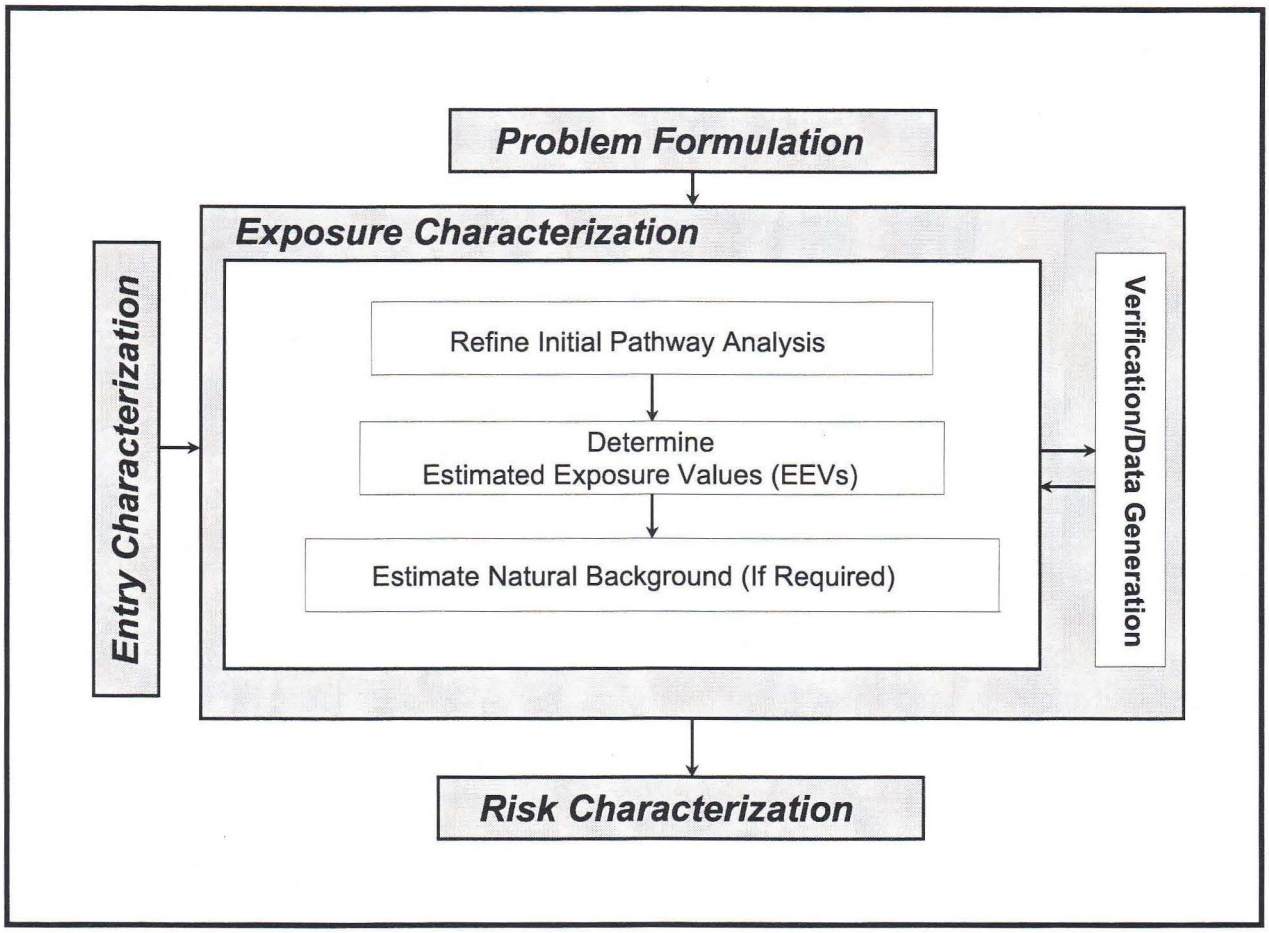

Figure 5.1 Exposure characterization in the ecological risk assessment framework for priority substances

Detailed pathways analysis may be qualitative, although quantitative analysis — using numerical models — is preferred. Regional multimedia fugacity models (e.g., Mackay *et al.* 1991; Cowan *et al.* 1995) could, for example, be used to predict the identity of environmental compartments in which organic substances accumulate. Single-medium models for air, surface water, groundwater, or soil (e.g., ECETOC 1992; Crowe and Mutch 1994) could also be used to predict environmental distribution on more local scales.[3] Food chain bioaccumulation models (e.g., Thomann 1989) could be used to estimate transfer of organic substances across several trophic levels. Experts should be consulted when using complex models.

[3] Guidance on the selection of such models may be found, for example, in U.S. EPA (1987, 1988, 1991).

Box 5.1 *Example of Qualitative Pathways Analysis*

A qualitative pathways analysis relating leakage from an above ground storage tank to exposure of organisms in a nearby stream could take the form of a statement that, because

- the concentration of a persistent substance in an aquifer below a leaking tank, used to store the substance, was observed to decrease with increasing distance from the tank, and
- the groundwater is flowing relatively rapidly towards the stream, and
- the substance was detected in the stream, below (but not above) the expected point of entry of the contaminated groundwater plume,

release of the substance from the tank and its dispersion in groundwater have resulted in exposure of organisms in local surface water.

When numerical modelling methods cannot be applied or are not required — because there are abundant field data, for example — pathways analyses may be expressed in conceptual terms (e.g., Box 5.1).

5.2.1 Verifying Pathways Analyses

Whenever possible, data on measured concentrations of the substance in areas and media of concern should be used to verify accumulations predicted by pathways analyses.

5.2.2 Quantifying Fate Parameters

Values assigned to key fate parameters may significantly affect pathways analysis. Values for such parameters, and their uncertainties (e.g., 95% confidence intervals), should be determined as accurately as possible, particularly when used in numerical fate or exposure models.

The physical and chemical properties of a substance, such as vapour pressure, partition coefficients, and aqueous solubility, can significantly influence its environmental fate. Accepted experimental methods of quantifying such properties are preferred (e.g., OECD 1993a); however, values calculated as described by Lyman *et al.* (1990) or OECD (1993b) may be acceptable.

Properties of the receiving media can also influence the behaviour, chemical form, and environmental concentrations of a substance. Parameters of possible importance include light intensity, pH, oxidation potential, temperature, intermedia partition coefficients, physical dimensions, and bulk densities of environmental compartments. When used in numerical models, values for key environmental properties and their uncertainties should, whenever possible, be based on field data from the area of concern.

The nature and rates of key transport and transformation processes affect the environmental persistence and possibly bioavailability of a substance. Transformation processes of potential importance include complexation, precipitation and dissolution, sorption and desorption, oxidation and reduction, hydrolysis, volatilization, photolysis, and biotransformation (e.g., Mill 1993; Hamelink *et al.* 1994). Rate values determined empirically using acceptable laboratory or field test methods (e.g., Knox *et al.* 1993; OECD 1993a) are preferred. If required, however, rates may be based on calculated values (e.g., OECD 1993b).

The extent to which a substance accumulates in organisms that serve as food sources for sensitive predators should be determined as bioaccumulation or bioconcentration factors (BAFs or BCFs). BAFs are the preferred measure of accumulation potential; however, BCFs are also acceptable, particularly when ingestion of food is not expected to be an important exposure route. BAFs are usually calculated from field data, whereas BCFs are normally determined experimentally. BCF test durations should be sufficient to achieve a steady-state concentration in the test organism (ASTM 1993; OECD 1993a). For organic substances, BCFs may also be estimated from QSARs or K_{ow} values (e.g., OECD 1993b). Because of the complexity of uptake processes, BAFs and BCFs for metal cations — especially for nutritionally essential elements — should be applied only to organisms and exposure conditions similar to those for which they were measured (CEU 1995; MMWG 1996).

5.3 Quantifying Exposure

Generally, exposure should be quantified as a distribution of empirically determined or calculated EEVs for each identified receptor in each area of concern.

5.3.1 Approaches to Quantification

EEVs may be based on concentrations of the substance in tissues of exposed organisms or on various measures of external exposure (Suter 1993). For dermal contact, EEVs may be expressed as concentrations in external media such as water or soil. In cases of exposure by ingestion or inhalation, EEVs should be determined as rates of intake. When more than one medium could contribute significantly to external exposure, EEVs should be calculated as the sum of intakes of all relevant media. In the case of radionuclides, the EEV will be the total dose of radiation. Total dose includes dose from radionuclides within the organisms (internal dose) and that received from radionuclides in the environment (external dose, e.g., in sediment and water). A computerized exposure model for organic substances developed by the Canadian Wildlife Service can be used to calculate multimedia exposures of birds, mammals, amphibians, and reptiles. Assessors should contact the Canadian Wildlife Service regarding its use. An example of output from this model is illustrated in Table 5.1.

Table 5.1 Estimated maximum total daily intake of hexachlorobenzene for a 1-kg adult mink in the St. Clair River area.

Medium	***Maximum Concentration***[a]	***Intake of Medium***[b]	***Maximum Daily Intake ($ng \bullet kg\text{-}bw^{-1} \bullet d^{-1}$)***
Air	0.29 $ng \bullet m^{-3}$	0.55 $m^3 \bullet d^{-1}$	0.16
Water	87 $ng \bullet L^{-1}$	0.1 $L \bullet d^{-1}$	8.7
Diet 1: 100% fish	283 $ng \bullet g^{-1}$	215 $g \bullet d^{-1}$	60 845
Diet 2: 100% birds or mammals	30 $ng \bullet g^{-1}$	158 $g \bullet d^{-1}$	4 740
Total Daily Intake — for Air, Water, and Diet 1			60 854
Total Daily Intake — for Air, Water, and Diet 2			4 749

[a] Concentration data were obtained from Health Canada and Environment Canada (1993), assuming that concentrations in birds and mammals are approximately equal. Note that bioavailability is not considered in this example.

[b] Methods of estimating intake of each medium are described in Moore *et al.* (1996).

EEVs for complex routes of exposure may be estimated as an internal dose using toxicokinetic models (Suter 1993). As explained in Chapter 5 of the resource document, although biomarker data may be used qualitatively, as part of the weight-of-evidence approach for estimating exposure to certain substances, biomarker measurements should not be used as surrogates for more conventional dose or concentration data.

5.3.2 Use of Field Data

EEVs, particularly those used in Tiers 2 and 3, should usually be based on results of monitoring studies undertaken in the areas of concern. Methods of sample collection, handling, storage, and analysis used in key studies should be carefully evaluated. Methods should, ideally, follow acceptable protocols, such as CCME

(1993). When chemical species are determined, changes in chemical form should be avoided. Methods should also avoid contamination or loss of analyte prior to or during analysis. Data on accuracy, precision, and detection limits of key analyses should be reviewed. To demonstrate accuracy, standard reference samples (e.g., Environment Canada 1995) may be analyzed; concentrations reported should be within the accepted range. Analytical precision or reproducibility is usually acceptable if results of repeated analyses of a typical sample are within 20% of the average value for the sample, at approximately the 95% confidence interval.[4] Less precise data may be acceptable in some circumstances, however. An analytical method is usually not acceptable if concentrations in most samples analyzed are below detection limits, and a more sensitive method should be sought. However, if detection limits are significantly lower than the ENEV, a "not detected" result may be useful.

Sampling and analytical strategies should ideally permit the characterization of spatial and temporal variations of exposure both in areas of concern and in appropriate background or reference locations.

EEVs should, to the extent possible, reflect current exposure conditions.[5] Therefore, exposure estimates are preferably based on data that are no more than a few years old. Older data may be acceptable when releases have not changed significantly over time and when:

- estimating exposure values for Tier 1,
- estimating levels of a persistent substance in media expected to remain compositionally stable for relatively long periods (e.g., some soils and sediments), or
- determining natural background concentrations of a substance.

5.3.3 *Use of Calculated Values*

Although EEVs that are directly measured are preferred, Tier 2 and 3 EEVs may be calculated by applying simple exposure conversion models to concentration data for key exposure media (Table 5.2). For example,

- equilibrium models (see Appendix II of the resource document) may be used to calculate concentrations of bioavailable forms of a substance,
- body burden values may be calculated as the product of measured concentrations in an exposure medium and a BAF, or
- total rate of intake may be calculated as the sum of measured concentrations in exposure media, including food, water, and air, multiplied by consumption rates (e.g., Table 5.1).

When concentration data for key exposure media are lacking, outputs from simple exposure models that have been adequately validated may be used to determine EEVs for Tiers 2 and 3, but only if the uncertainties associated with calculated exposure values are small (Table 5.2). An example would be a dilution model, where a measured concentration in an effluent is divided by a dilution factor. When there is significant uncertainty associated with model outputs (e.g., for more complex fate and exposure models that have not been adequately fiel tested), results should be used only to complement empirical data, as part of a weight-of-evidence approach to quantifying exposure. Tier 1 is exceptional, however, in that EEVs may be based entirely on complex or uncertain model predictions, but only models have been properly validated and when conservative assumptions are made about exposure parameters (Table 5.2).

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[4] Precision is sometimes also expressed as a coefficient of variation. The coefficient of variation that corresponds to a precision of 20%, at approximately the 95% confidence level, is 0.1.

[5] It is not necessary, however, that EEVs reflect current environmental loadings. For example, EEVs based on concentrations of persistent substances in recent samples of soil and sediment may be more reflective of historic than of current emission rates.

Table 5.2 Guidance on application of tiered approach to quantifying exposure.

Tier	Representation of EEVs		Average Exposure over Time or Home Range	Models		Treatment of Bioavailability
	Empirical Data	**Monte Carlo Simulations**		**Acceptable Types**	**Conservatism of Parameter Values[a]**	
1	measured maximum value	99.9th percentile value	no	simple or complex	highest	assume maximum bioavailability
2		95th percentile value	possibly	only simple models or Monte Carlo-type simulations[b]	intermediate	use best estimate of bioavailability
3	distribution of values				lowest	

[a] For example, BCFs, rate constants, etc.

[b] Outputs from more complex exposure models may be used to support empirical data.

As indicated in Chapter 7, Monte Carlo methods may be used to derive distributions of EEVs for Tier 3, when EEVs are calculated as a function of two or more exposure variables represented as distributions (e.g., distributions of concentrations in food and of food intake rates).

5.3.4 Determining Bioavailability

In order to compare critical exposure and effects data, the bioavailability of the substance in both data sets should be similar (CEU 1995). Generally speaking, toxicity studies are conducted under conditions that maximize bioavailability. For example, studies with aquatic organisms are typically conducted using soluble forms of a substance (e.g., a soluble metal salt) in test water that is free of the dissolved organic matter and suspended solids that commonly reduce bioavailability in natural waters.

Consequently, for Tiers 2 and 3, EEVs should generally be based on concentrations of bioavailable forms of substances. For some substances, it may be appropriate to normalize EEVs — and CTVs — to parameters that control bioavailability, such as organic carbon or water hardness. Tier 1 is exceptional, however, in that maximum bioavailability may be assumed (Table 5.2). For example, the total concentration of a metal in soil may be used to determine an EEV for Tier 1, even though only a small fraction of the total may be available for uptake by soil organisms.

Body burden data are the preferred measure of exposure to bioavailable forms of substances that are not significantly metabolized, but only when complementary effects data are available (McCarty *et al.* 1992). This is because body burdens integrate the effects of differing exposure conditions and assimilation processes (Landrum *et al.* 1992). Furthermore, it is the accumulation of a substance at a sensitive target site within an organism that is responsible for its harmful effects (McCarty 1987).

Tissue concentrations may be based on analysis of a whole body or individual organs. Information on the mechanism of action and pharmacokinetic properties of the chemical/organism combination is needed to determine whether specific organs or whole-body burdens should be used (Norton 1996).

It may be appropriate to normalize whole-body burdens of hydrophobic substances, with relatively rapid excretion rates, to lipid contents (Gobas and Mackay 1989).[6] This is less appropriate for very slowly excreted chemicals with depuration rates lower than growth rates (e.g., Borgmann and Whittle 1992). As whole-body data on the metal content of organisms may not be indicative of potential biological effects (Hare 1992; Cain *et al.* 1995), data on metal levels in specific tissues (e.g., bone or blood) or cell components (e.g., cytosol) may be preferred.

When data on metal concentrations in tissues are lacking, values may be calculated using empirically derived regression equations (e.g., Box 5.2). These typically relate concentrations of a metal in organisms to levels in exposure media and to those physical and chemical properties of the media that determine bioavailability, such as pH and clay or organic matter content. Because of their empirical character, such regressions should not be applied to organisms or environmental conditions that differ significantly from those for which they were developed. Furthermore, because of their large uncertainties, they should generally be used only to estimate exposure for Tier 1 or to complement empirical body burden data for Tiers 2 and 3.

When body burden data cannot be used, exposure to bioavailable forms of a substance may be determined based on concentrations of dissolved or "soluble" forms of the substance in key exposure media — including pore waters of sediments or soils.

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[6] This is most appropriate when lipid contents are high and easy to measure (e.g., >3–5%). Otherwise, large experimental errors may be introduced into exposure measurements (Lanno 1996).

Bioavailable forms of substances should be determined on a case-by-case basis, depending upon the nature of the substance and the assessment endpoint(s). In the case of organic and metallo-organic compounds, un-ionized,[7] freely dissolved forms are primarily available for uptake (Suffet *et al.* 1994). For metals, the concentration of the freely dissolved "aquo ion" (e.g., $Zn(H_2O)_6^{2+}$) is often the best indicator of metal bioavailability (Benson *et al.* 1994; Campbell 1995). However, oxyanions are also taken up by organisms (Benson *et al.* 1994), and there is evidence that some dissolved organic and inorganic metal complexes are bioavailable (Campbell 1995).

Box 5.2 *Empirical Relationships Between Uptake of Substances, Exposure Concentrations, and Properties of Exposure Media*

Regression methods may be used to relate data on concentrations of a substance in organisms to concentrations of the substance in an exposure medium, as well as to physical and/or chemical properties of the medium that determine bioavailability. For example,

- the metal content of plants (M_{plant}) may be related to the HCl-extractable metal content of the supporting soil (M_{soil}), as well as its pH and clay and organic matter (OM) content, as follows:

$$M_{plant} = a(M_{soil}) + b(pH) + c(\%clay) + d(\%OM) + e$$

where a, b, c, d, and e are empirically derived coefficients, or

- the metal content of molluscs ($M_{mollusc}$) may be related to the H_2O_2-extractable metal content (M_{sed}) and organic carbon (OC) content of host sediment as follows:

$$M_{mollusc} = a[M_{sed} \cdot (\%OC)^{-1}]$$

where a is an empirically derived coefficient.

The above was adapted from Martens (1968) and Tessier *et al.* (1984), respectively.

Methods that can be used to directly measure concentrations of various dissolved forms of both organic and inorganic substances are described in Suffet *et al.* (1994) and Pickering (1995) (see Appendix II of the resource document). When there are no empirical data on specific bioavailable forms, equilibrium models may be used to estimate concentrations of dissolved species (see Appendix II of the resource document). For example, MINEQL+ (Schecher and McAvoy 1994) could be used to calculate concentrations of different dissolved metal species from total concentrations in unfiltered water samples and data on the nature and amounts of other dissolved and solid phases.[8] Similarly, the EqP model of Di Toro *et al.* (1991) may be used to estimate concentrations of the freely dissolved form of a neutral organic compound in the pore water of a sediment, if its concentration and that of organic carbon in the solid phase of the sediment are known.

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[7] Ionized forms of organic compounds are not entirely unavailable for uptake by organisms. For example, organic cations can (to some extent) partition to lipid phases, especially for chemicals that have neutral forms that are strongly hydrophobic (Erickson *et al.* 1994).

[8] Equilibrium modelling should be applied only to systems containing metal-complexing ligands with known thermodynamic stability constants (Turner 1995).

Exposure to "soluble" solid forms of metals and metalloids in solid phases can be measured using chemical reagents that remove the more weakly bound forms of the substance (see Appendix II of the resource document). Reagents should be selected carefully, taking into account the nature of the substance and the conditions of exposure. Box 5.2 presents examples of two such reagents used to estimate the fractions of bioavailable metal in soils and sediments.

When exposure is estimated as rates of intake (e.g., Table 5.1), bioavailability factors (ranging from 0 to 1) may be applied to total intake values for individual exposure media. Bioavailability factors for ingested and inhaled solids may be estimated using weak acid extractions intended to simulate conditions in the gastrointestinal tract (metals only) or using data from assimilation studies with laboratory organisms (e.g., Borgmann and Whittle 1992; Stern 1994; Fisher and Reinfelder 1995).

For some substances, bioavailability is controlled by a specific chemical component of an exposure medium. Concentrations of such substances may be adjusted or normalized to the controlling variable. For example, uptake of metal ions from solution may be reduced by competition for adsorption sites on the surface of exposed organisms from calcium and magnesium (i.e., hardness) ions (Campbell 1995). In this case, EEVs — and CTVs — could be adjusted to hardness, as described by Parkhurst *et al.* (1994). Similarly, the bioavailability of nonionic organic substances in sediment is often inversely related to the abundance of organic carbon (Di Toro *et al.* 1991). Differences between bioavailabilities in sediment used for toxicity testing and field sediments may therefore be minimized by normalizing total concentrations of nonionic organic substances in sediments to their total organic carbon contents.[9]

5.3.5 Representation of Temporal and Spatial Variability

EEV distributions may reflect both spatial and temporal variability of exposure, as well as uncertainties associated with exposure measurements and — when EEVs are calculated— ignorance of true values for key parameters (e.g., K_{ow}, BAF) used in calculations (Hoffman and Hammonds 1994).

As indicated in Table 5.2, the measured maximum EEVs should be used as numerators in risk quotients for Tier 1 risk estimates. If EEVs are based on Monte Carlo analysis, the 99.9th percentile EEV may be conservatively chosen as a "bounding estimate" of exposure (U.S. EPA 1992). For Tier 2 risk analyses, a less conservative value, such as the 95th percentile, should be used.[10] Tier 3 analyses make use of entire EEV distributions. In some circumstances (see below), EEVs may represent averaged exposure values.

For Tier 3, spatial and temporal variations in exposure values should be separated whenever possible. In such instances, EEVs may take the form of frequency distributions that reflect the variability of exposures at the same time but at different locations or at different times at a particular monitoring station. If sample locations are selected at random and organisms are assumed to be uniformly distributed within the sampled area, EEV distributions representing spatial variability can be used to estimate the proportion of the population of receptors that are exposed at levels above the ENEV (see Chapter 7). If sampling times are selected appropriately, temporal EEV distributions may be used to estimate the proportion of time that exposure values exceed the ENEV at a particular monitoring station.

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9 Limitations of this approach have been discussed by Landrum and Robbins (1990).

10 As explained in U.S. EPA (1992), Monte Carlo simulations often include low-probability estimates at the upper end of the exposure range that are higher than those actually experienced in a population.

For discontinuous exposures, the timing, duration, and frequency of exposure are important. Timing may be a key determinant of exposure for organisms with seasonal migration patterns or with sensitive life stages. In such cases, EEVs should be based on data for times when receptors are likely to be exposed to the substance or are particularly sensitive to the substance (e.g., during spawning).

Temporal Variability

Generally, exposure at a particular location is characterized by estimating arithmetic average exposure values for a specified time interval, such as a day or month.[11] The selection of an appropriate time interval depends upon whether exposure is episodic or continuous and upon the acute or chronic nature of the assessment endpoint. Short exposure averaging periods are used when exposure is episodic or assessment endpoints are acute. Longer periods should be used with chronic assessment endpoints. Whenever possible, time intervals should be matched to exposure periods used for determining effects (e.g., Solomon *et al.* 1996).[12] For example, if the exposure period used in a critical toxicity experiment was four weeks, individual exposure values should ideally represent four-week averages.[13]

When samples have been collected frequently over an extended time at the same site, the sampling period may be divided into appropriate time intervals, and concentrations in samples from each time interval may be averaged (e.g., Solomon *et al.* 1996). In such cases, the maximum concentration in a single sample is used as a Tier 1 EEV; for Tiers 2 and 3, however, the maximum EEV and the EEV distribution should generally be based on moving-average or time-averaged concentrations (Table 5.2).

If exposure values are based on infrequent sampling of mobile media such as air and river water, variations in intensity of sources and flow and dilution characteristics must be considered when determining if such data are representative. EEVs based on one-time or short-duration sampling of relatively immobile media, such as soils and sediments, may often be assumed to represent longer exposure periods, if a substance is persistent.

Spatial Variability

Tier 3 EEV distributions reflecting spatial variations in exposure are often intended to reflect the variability of exposure of individual organisms within a population (U.S. EPA 1992). To determine the exposure of individuals when assessment endpoints are chronic, spatial variations in exposure values may be averaged over areas that correspond to the expected "home range" of individual organisms. Home ranges of fish and mammals, for example, can be estimated as an allometric function of body size (e.g., Minns 1995). Areas involved could be as small as a few square metres for small immobile organisms or as large as hundreds of square kilometres for large mammals.

When samples have been collected at many sites over a large area, home range-size subareas may be defined and concentrations in samples within each subarea averaged. In such cases, the maximum concentration in a single sample is used as a Tier 1 EEV; for Tiers 2 and 3, on the other hand, the maximum EEV and the EEV distribution may be based on spatially averaged concentrations (Table 5.2). Spatial averaging may be difficult, however, because of limited knowledge of the distribution of organisms within specific areas of concern and the limited sample densities of most field surveys. Consequently, Tier 3 EEV distributions are often based on "raw" or spatially unaveraged exposure data. When

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[11] Although median or geometric mean concentrations may be better estimates of "typical" concentrations, these statistics may downplay the importance of the highest concentrations, which are probably the most toxicologically significant (Norton 1996).

[12] Such matching would not be appropriate, however, when chronic effects levels are estimated from acute toxicity data.

[13] If required for Tier 3 analysis, confidence limits may be estimated for average exposure values (e.g., Dixon and Massey 1969).

interpreting EEVs based on such "raw" data, it should be recognized that there will be a tendency to overestimate the proportion of a population that is exposed at high concentrations (Hattis and Burmaster 1994).

5.4 Estimating Natural Background Concentrations

Information on natural contributions to EEVs may be required to establish lower bounds on ENEVs for natural substances and to evaluate the potential for natural tolerance in receptor organisms (see Chapter 7).

Methods that may be used to distinguish between natural and anthropogenic components of measured EEVs are described in Section 5.7 of the resource document. Methods may be simple, such as comparing concentrations of a substance in an exposure medium to distance from a point source (e.g., Freedman and Hutchinson 1980). Alternatively, more complex receptor models (e.g., Gordon 1988) or specialized statistical or chemical methods (e.g., Forstner 1983; Maenhaut *et al.* 1989) may be used. Although quantitative results are preferred, there are often large uncertainties associated with estimates of natural background concentrations for anthropogenically contaminated areas. Consequently, several methods should be applied whenever possible, using a weight-of-evidence approach.

5.5 Some Points to Remember

- Clearly describe the purpose and scope of the exposure characterization and underlying methodologies.
- Critically evaluate exposure data and express the degree of confidence in the data. Present the rationale for excluding data.
- If exposure models are used, describe their benefits, weaknesses, and limitations.
- Describe the central estimates and upper and lower confidence limits on exposures; note and support the use of any preferred estimates.
- Describe uncertainties in exposure estimates, and highlight the relative importance of key assumptions and data.
- Describe research or data necessary to improve the exposure assessment.

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CHAPTER 6

EFFECTS CHARACTERIZATION

6.1 Introduction

6.1.1 Goals and Objectives

The objective of the effects characterization phase is to define a CTV for each assessment endpoint. The results of toxicity studies on the most sensitive measurement endpoint are used to derive a CTV. A CTV is usually an estimate of low toxic effect, such as an IC_{25} or LOEL, and may be in the form of a point estimate for Tiers 1 and 2 or a distribution for Tier 3, such as $IC_{25} \pm 95\%$ confidence limits. Section 6.3 provides guidance on deriving CTVs. Chapter 7 describes the approaches to be used for deriving an ENEV from a CTV.

6.1.2 Relationship with Other Phases

The effects of a substance on assessment and measurement endpoints identified during problem formulation are determined during the effects characterization stage. It is important that effects on sensitive receptors be identified as assessment endpoints. This is particularly important for uptake models that require input parameters, such as ingestion rates or inhalation rates, that differ for each receptor. It may become apparent that the assessment and measurement endpoints originally identified are not appropriate. This would be the case, for example, if the results of toxicity studies show that other types of organisms are more sensitive than previously believed or if the results of detailed exposure characterization indicate that the substance partitions to media other than those originally identified during problem formulation. In such cases, problem formulation would have to be revised and different endpoints identified.

Once CTVs for the appropriate assessment endpoints are determined, they are used as inputs to the next phase of the risk assessment, the risk characterization phase (Figure 6.1).

6.1.3 Overview of Approach

Toxicity information should include data from a wide range of trophic levels. These help determine which populations, communities, and ecosystem processes may be particularly susceptible to adverse effects, as well as the types and magnitude of these effects. Assessors should attempt to locate data pertaining to Canadian species and conditions whenever possible.

Available toxicity studies are critically evaluated, and only studies of acceptable quality are given further consideration (Appendix III of the resource document; Environment Canada 1996). Assessors should be aware that the toxicity of substances can be modified by various environmental conditions (e.g., temperature, water hardness, etc.) and by characteristics of the biota (e.g., species, age, behaviour, interaction among species) (Environment Canada 1996). Assessors should consult standard protocols for guidance on acceptable studies. If no acceptable studies are available, research may need to be carried out to supply the required information.

Where necessary, the results from acceptable studies are refined to yield the type of experimental endpoint required. In order of preference, these are IC_{25}, LOEL, NOEL, EC_{50}, or other measure of central tendency (see Section 6.3).

Assessors should identify sources of uncertainty, both qualitative and quantitative, related to toxicological data (see Section 6.3 of the resource document). This will be taken into account at the risk characterization phase in selecting the appropriate application factor or in a quantitative uncertainty analysis. Areas of concern include uncertainties regarding the relationship between the substance and the assessment endpoint, uncertainties associated with parameters in the studies, and natural variations in relevant media and biological effects. In the case of radionuclides, areas of concern include uncertainties regarding the relationship between whole-body doses and doses to sensitive tissues and organs, uncertainty in dosimetry models for nonhuman species, and uncertainty in the most appropriate factor to take into account for the relative biological effectiveness (RBE) of alpha emitters.

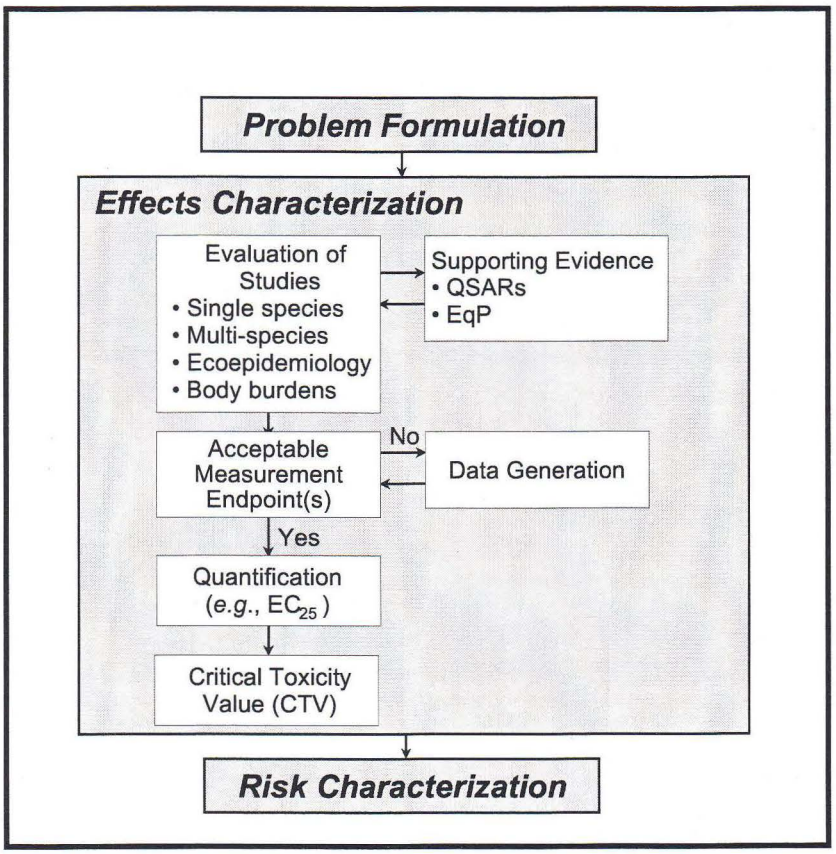

Figure 6.1 Effects characterization in the ecological risk assessment framework for priority substances

6.2 Types of Effects Information

Studies on single species, multiple species, ecoepidemiology, body burdens, QSARs, and the EqP method can all be used to characterize effects on the assessment endpoints of concern. Depending on the substance being assessed, several of these types of studies can be used. The limitations of each, however, should be considered. Types of effects data required for each tier will depend on the exposure scenario of the substance in the environment. In order to minimize the degree of uncertainty involved in extrapolation, the measurement endpoints selected should be as relevant as possible to the exposure scenarios. For example, if the substance is introduced into the environment in a pulsed or intermittent way and is not persistent, then short-duration (acute) tests should be used in deriving the CTV for each tier. For substances that are continuously released into the environment or are persistent, chronic studies are preferred. All acceptable studies contribute to an understanding of a substance's effects. The most relevant studies contribute directly towards the determination of CTVs. These studies should use species found in Canada or closely related species. They should be from a range of trophic levels and represent a variety of exposure routes.

Full life cycle studies that determine effects on embryonic development, hatching success, survival of juvenile stages, growth, reproduction, and survival of adults are preferred. In their absence, results may be employed from partial life cycle studies using the most sensitive stages of the life cycle (OECD 1993a). If there is only one study, assessors will have to decide on a case-by-case basis whether it provides sufficient information to establish that there are adverse effects on the assessment endpoint. The purpose of these studies is to determine if there is sufficient

information to establish whether there is an effect on the assessment endpoint based on data from the measurement endpoint.

6.2.1 Single-Species Toxicity Tests

Single-species toxicity tests determine the effects of substances on organisms of a single species under specified test conditions. Such tests are needed to obtain information about the concentrations of substances and durations of exposure that cause changes in the survival, reproduction, growth, physiology, biochemistry, or behaviour of individuals within particular species (Cairns 1983). Biochemical or physiological perturbations may also have implications for population effects (Section 1.2). Such effects at lower organization levels include endocrine disruption (Colborn *et al.* 1993), genotoxicity (Anderson *et al.* 1994), and immune suppression. Standard measurement endpoints are available for some of these examples (OECD 1993a; Kramer and Giesy 1995).

The usefulness of single-species tests for predicting effects depends on the degree to which predictions can be extrapolated to natural systems with confidence and the tests' replicability and reproducibility (Cairns 1992). Single-species toxicity tests make it easier to determine the direct effects of varying individual test conditions. These effects may be masked by interactions among species or environmental components in microcosm or mesocosm tests. Standardized test methods developed by agencies such as Environment Canada, the U.S. EPA, and the OECD have enhanced the likelihood of achieving reproducible results when single-species tests are carried out by researchers in different laboratories. If other test methods are used, the procedures must be described in sufficient detail that the reliability of the results can be judged.

When using single-species laboratory tests for assessing risk, the following points should be kept in mind. Physiological or biochemical variations among species, such as uptake and metabolism, can alter the potential toxicity of a substance. Inbred laboratory strains may be unusually sensitive or resistant to the test substance. Single-species tests are often unable to accurately predict effects at higher levels of ecological organization, where population dynamics such as age structure and density may have an effect. Alterations in ecosystem characteristics, such as changes in community function, energy flow, and nutrient cycling, cannot be predicted from single-species tests (Cairns 1983). Unlike many microcosm and mesocosm tests, single-species toxicity tests are not designed to integrate the simultaneous study of toxicity and various chemical transformation and partitioning processes. Behavioural and ecological parameters, such as competition and seasonal changes in temperature, may affect a species' sensitivity to a substance. Application factors may account for uncertainties, and quantitative uncertainty analyses may estimate many of these uncertainties (Chapter 7). Ideally, risk assessors should rely on a number of single-species *and* multispecies toxicity tests. The two types of tests complement each other and present a more accurate characterization of effects than either type used alone.

6.2.2 Multispecies Toxicity Tests

Multispecies toxicity tests, including microcosm, mesocosm, and field tests, incorporate ecological components (species, functional groups, or habitat types) that simulate processes as they occur in nature (SETAC 1992). A microcosm can range from a small laboratory-scale simulation of a portion of an ecosystem to a large outdoor tank. A mesocosm can range from laboratory microcosms to large, complex ecosystems (Grice and Reeve 1982; Odum 1984). Mesocosm tests, generally performed outdoors, more closely approximate natural ecosystems than do microcosm tests (Taub 1985). Field tests, once considered as large mesocosms, normally involve the isolation of terrain or part of a body of water and include within their boundaries the normal flora and fauna found under unperturbed conditions.

There are few examples of protocols for standardized microcosm tests for aquatic and terrestrial systems. Several aquatic mesocosm test protocols have been described in the literature (Touart 1988), and terrestrial mesocosms have been used for several decades (Barrett 1968). Field tests can confirm whether predicted fate, chronic effects, or bioaccumulation actually occur under reasonably realistic field conditions. They can also reveal secondary effects that result from species interactions (OECD 1995).

Multispecies tests may not be as useful at demonstrating ecosystem recovery processes following a spill or stress as suggested by Harrass and Sayre (1989). In fact, Power (1996) indicates that both Cairns (1990) and Detenbeck *et al.* (1992) have shown that recovery is very difficult to demonstrate in a model ecosystem. Following disturbances in the natural environment, there are site-specific factors affecting rates of recovery, such as immigration rates from undisturbed areas, that are difficult or impossible to reproduce in a microcosm. Multispecies tests may be particularly useful in the ecological assessment of complex mixtures and effluents (Chapter 8). Harrass and Sayre (1989) suggest that acceptable multispecies test data include three key features: *credibility*, *applicability*, and *endpoint interpretability* (Section 6.2.2 of the resource document). Assessors should ensure that these features are included in multispecies test protocols.

Microcosm experiments, like single-species tests, are not globally sensitive to all stresses. When microcosms lack appropriate target species for substances with specific modes of action, little effect will be detected (Pratt *et al.* 1993). Toxicity to individuals, as measured by single-species tests, is not always reflected in toxicity to populations, and population interactions tend to dampen responses at the community level (Koojiman 1985). Complex interactions can vary from one system to another, so that meaningful differences are often obscured. Assessors should be cautious in making projections to ecosystems based on these tests (Odum 1984). Population dynamics, such as compensatory mortality mechanisms, play a pivotal role in attenuating the impact of many stresses. This capacity is limited, and, thus, accurate effects assessment requires detailed knowledge of the suite of stresses acting on a population (Power and Power 1995). Microcosms require a period of stabilization for component species, and microcosm tests are much more costly than single-species toxicity tests (U.S. EPA 1992a). Natural communities are often difficult to sustain in an artificial arrangement. There may be extinctions and changes in community structure irrespective of substance exposure (Buikema and Voshell 1993).

6.2.3 *Ecoepidemiology*

Ecoepidemiology attempts to determine the causes of observed effects in the field by examining the spatial and temporal relationships between these effects and suspected causal agents (e.g., PSL substances). Effects of concern include diseases in individuals and populations, disturbances in communities, and disruptions of ecological systems. In most risk assessments, laboratory toxicity data are used to predict adverse effects on the environment, whereas ecoepidemiology starts with observed field effects and attempts to identify causes. Epidemiological criteria may be used in conjunction with other laboratory-derived information to determine the potential of substances to cause adverse effects.

Ecoepidemiology may prove especially useful in assessments of complex mixtures, where direct cause-and-effect relationships are difficult to ascertain in the laboratory (Chapter 8). Confidence in causal relationships can be increased by selecting reference sites and evaluating changes along a concentration gradient where differences in other environmental factors are minimized (U.S. EPA 1992b).

Statistical associations derived from well-controlled experimental studies can aid in establishing causal relationships even when the causative agent has not been demonstrated conclusively. Confounding factors that can obscure a substance's effects include differences in habitat quality between areas, natural variations in environmental parameters within areas, the occurrence of undetected stressors, and the movement of organisms into or out of the study area (U.S. EPA 1992b).

Results of the ecoepidemiology method will often be inconclusive. The best that can be expected is to reach the most reasonable explanation based on the evidence at hand. In ecoepidemiology, most studies are observational, and experiments to confirm cause-and-effect relationships may be difficult or impossible to carry out.

Ecoepidemiology has the same basic principles as epidemiology. Fox (1991) has adapted criteria to help assess the relationship between a suspect substance and an adverse environmental effect (see Section 6.2.3 of the resource document for a

complete listing). Although these criteria do not provide proof of a cause-and-effect relationship, they do provide a process and framework upon which to exercise judgment.

6.2.4 Estimating Effects of Naturally Occurring Substances

Organisms resident in areas where natural background concentrations of a naturally occurring substance are elevated are likely to have acquired a tolerance for that substance. Toxicity tests using standard laboratory strains would therefore not be directly applicable to these organisms. CTVs should ideally be based on single- or multispecies tests or on field tests using organisms collected from the areas with naturally elevated background concentrations. When this is not practical, CTVs should be derived from tests with organisms with tolerances matched as closely as possible to those of risk receptors.

6.2.5 Critical Body Burdens (CBBs)

CBBs are the minimum tissue concentrations that are associated with an adverse effect on a measurement endpoint C the reproductive potential of *Daphnia*, for example. Traditionally, results from acute and chronic toxicity tests are expressed in terms of the concentration in the external medium in relation to the biological response or measurement endpoint. The CBB method, which is based on whole-tissue concentrations or the concentration in a particular target organ, can be an effective surrogate for the target site(s) of action. It can provide a more direct measure of a predicted adverse effect than can an external exposure concentration C such as single-species testing C as problems associated with estimating bioavailability and accumulation are essentially eliminated.

When appropriate, CBBs should be summarized and compared with tissue residue or body burden data collected in the field. This information may be used as the basis for the risk assessment or to support a weight-of-evidence approach for other analyses, such as the external concentration method. Although CBBs of organic substances have been linked to the acute toxicity of narcotics in aquatic organisms, more research is required before this concept can be generally applied to other modes of toxic action (McCarty and Mackay 1993).

Assessors should use body burden data and, where possible, CBBs, along with more traditional toxicity information, in characterizing effects in both the aquatic and terrestrial compartments. If research is required to fill data gaps, CBBs should be measured during standard toxicity bioassays. This reduces uncertainties in comparing field and laboratory data relating to bioavailability, exposure routes, and intake rates.

CBBs may be especially useful for assessing complex mixtures. Narcotic substances are essentially of equal strength on a molar residue basis, and, therefore, the toxicity of mixtures of these substances is additive. Based on this additivity theory, acute lethality occurs if the sum of the chemical concentrations in the organism reaches a threshold (effects) level (McCarty and Mackay 1993).

6.2.6 Quantitative Structure–Activity Relationships (QSARs)

In the absence of empirical data, QSARs may be used to predict effects of chemical substances. QSARs may also be used to determine the physical and chemical properties of a substance. QSARs are developed for groups of substances that are differentiated by mode of action, which varies with the structure and physicochemical properties of the substances, or by chemical class (e.g., chlorinated phenols, nonionic surfactants, phosphate esters). QSARs are applicable *only* to substances within that group.

QSARs can be used to make preliminary estimates of toxicity in problem formulation, to corroborate empirical data, and to determine the need for additional testing. QSARs are also used as supporting lines of evidence for estimating CTVs and should not be the primary source of evidence.

Two QSAR programs, ECOSAR and TOPKAT, are widely used for health and environmental assessments. The CEU (1995) also uses QSARs for aquatic toxicity tests (Section 6.2.5 of the resource document).

ECOSAR, developed by the U.S. EPA, uses over 100 QSARs for 40 chemical classes to predict acute and chronic toxicity to fish, *Daphnia*, and green algae as well as 14-day LC_{50}s for earthworms in artificial soil (U.S. EPA 1994). Approximately 50% of the QSARs are for neutral

organic chemicals. The remainder are for ionizable organic chemicals such as amines, phenols, or anilines.

TOPKAT, developed by Health Designs, Inc. (HDI 1990), uses structure–activity relationships and statistical techniques to estimate various effects, including *Daphnia magna* EC_{50}s and fathead minnow LC_{50}s.

Other QSAR programs could also be used for assessment purposes. The OECD (1993b) recommends the following:

- The substance under investigation and those used in the QSAR should be similar in terms of structure and mode of action.
- Only QSARs that have been verified in terms of range of application and predictive capability should be used.
- A detailed description of the domain of the QSAR should be provided. This includes the structural rules defining the group of substances and the ranges of the parameters for which the QSAR is valid.
- The data used to develop the QSAR should be described or referenced.

QSARs that fail to meet these criteria may still be useful, but they should be applied with particular caution. When the need for QSARs is identified, assessors should consult with experts to verify the predicted effects of these models.

6.2.7 Equilibrium Partitioning (EqP)

The EqP method estimates effects levels for benthic, soil-dwelling, and groundwater organisms exposed to hydrophobic, nonpolar, nonionic organic substances (Di Toro *et al.* 1991; van de Plassche and Bockting 1993). This method defines the chemical activity of the substance to which the resident biota are exposed by assuming chemical equilibrium between pore water and organic carbon in solid phases. It also assumes that water column organisms and those in the contaminated medium are equally sensitive to the substance. The advantage of this method is that effects values can be calculated quickly using effects data for water column organisms if the K_{ow} of the substance and the organic carbon content (K_{oc}) of the solid medium are known. However, the uncertainties associated with this method's basic assumptions can often limit its usefulness (Chapman 1989). For example, the method assumes:

- that the concentration of the substance in biota resident in the medium (i.e., a contaminated sediment, soil, etc.) is in equilibrium with concentrations in the aqueous and solid phases (Di Toro *et al.* 1991),
- that water column organisms and organisms in the contaminated medium are equally sensitive to the substance (Di Toro *et al.* 1991), and
- that dermal contact is the primary route of exposure and that exposure via ingestion of solid phases is not significant (Chapman 1989).

Despite the uncertainties surrounding these assumptions, effects values derived from the EqP method may be useful as screening values for problem formulation. Such data can also contribute to a weight-of-evidence approach for selecting a particular CTV for Tier 2 risk analysis.

6.3 Deriving Critical Toxicity Values (CTVs)

The concentration–response curve describes the response of individuals, populations, or other biological systems to a range of concentrations of a substance. For most priority substances, concentration-response curves will be available for a variety of endpoints and experimental conditions. Previous sections of this chapter describe how to select and evaluate studies as part of an effects characterization. The next step is to derive the CTV (see Appendix I for definition). A CTV is usually an estimate of low toxic effect (e.g., LOEL, IC_{25}) and is a point estimate for Tiers 1 and 2. For Tier 3, the objective is to derive a distribution for the CTV (e.g., $IC_{25} \pm 95\%$ confidence limits, concentration-response curve with confidence limits). In stating the CTV, assessors should indicate the type of result, the organism involved, and the duration of the test. In this manual, acute tests refer to tests with an exposure duration that is a small portion of the test organism's life cycle. Chronic tests may be partial or full life cycle tests. Quantal effects are referred

to as lethal concentrations (e.g., LC_{50}) or as effective concentrations if the effects are categorical but nonlethal (e.g., EC_{50} for immobilization of *Daphnia*). Quantitative effects (e.g., biomass, growth rate) are referred to as the inhibiting concentration for a (specified) percent effect (i.e., IC_p). This section outlines the preferred approaches and methods for quantifying CTVs. Detailed descriptions of preferred approaches and methods are provided in Section 6.3 of the resource document.

6.3.1 Tiers 1 and 2

CTVs used in Tier 1 and 2 assessments may be derived by several methods. In order of preference, they are:

(1) LC_{25}, EC_{25}, or IC_{25}

Recent publications have strongly recommended the use of a regression-based approach for deriving estimates of low toxic effects (e.g., Pack 1993; Noppert *et al.* 1994; Chapman *et al.* 1996; Environment Canada 1996; Suter 1996). Low toxic effects are preferentially determined from the results of chronic toxicity tests, except for substances that are present in the Canadian environment only for short durations. This approach generally requires five or more treatments and involves specifying a model and estimating its parameters through regression analysis. The desired point estimate is then determined by interpolation or extrapolation (see Section 6.3.3). As point estimates of low toxic effects are likely to be model dependent when toxicity results are extrapolated to the extremes of the curve (e.g., ≤ 5% effect) (Sebaugh *et al.* 1991; Moore and Caux 1997), we recommend a cutoff of 25% effect for Tiers 1 and 2; the estimate could be lower (e.g., IC_{10}) if it is the result of interpolation.

(2) LOEL or NOEL

Analysis of variance (ANOVA) has been the most common method of estimating low toxic effects from chronic tests. There are several reasons for this, including wide availability of software capable of performing ANOVA and related nonparametric tests and familiarity with the technique in the regulatory community. Also, most toxicity-testing protocols specify experimental designs more suited to hypothesis-testing methods such as ANOVA than to regression-based approaches. Nevertheless, hypothesis testing as an approach for estimating low toxic effects has a number of shortcomings, including the following: (i) NOELs and LOELs are test concentrations that do not correspond to specified effects levels from one test to the next, (ii) poor experimental design will mistakenly indicate that a substance is less toxic than it really is, and (iii) most information from the toxicity test is not used (Stephan and Rogers 1985; Pack 1993; Suter 1996). As a result, hypothesis testing is not the preferred method for estimating low toxic effects, particularly for Tier 2 assessments. If a LOEL or NOEL is to be used as the CTV, information regarding the minimal difference required to give a significant result should be provided (number of replicates, test variance, α, β, test concentration intervals). This is important, given that conventional hypothesis testing will usually determine a NOEL and LOEL, even with poor concentration-response data (meaning that effects >25% may not be detected as significant) (Stephan and Rogers 1985; Suter *et al.* 1987; Moore and Caux 1997). LOELs are preferred to NOELs in deriving a CTV, except when the LOEL represents a severe effect (e.g., >40% effect). In the latter case, NOELs are preferred. Maximum allowable toxicant concentrations (MATCs) are not used to derive a CTV.

(3) Median Toxic Effects

Tier 1 and 2 assessments may use estimates of median toxic effects derived from acute toxicity tests as CTVs, although it is the least preferred approach. Larger application factors are required to convert a CTV derived from a median toxic effect to an ENEV than is the case with a CTV derived from a low toxic effect.

6.3.2 Tier 3

The objective of a Tier 3 assessment is to estimate the probabilities of specified effects or a range of effects. If the objective of the assessment is to estimate the probability of exceeding a specified effect (e.g., 25%), then the CTV should include both the point estimate and the fiducial confidence limits (e.g., $IC_{25} \pm$ 95% confidence limits) (see Section 6.3.4 of the resource document). Note that this is possible only using a regression-based

approach (e.g., IC_{25}), as it is not possible to calculate confidence limits for a LOEL or NOEL. If the objective is to estimate the probabilities of a range of effects, then the CTV should include the entire concentration-response curve with confidence limits.

In some cases, the objective of a Tier 3 assessment may be to estimate effects at the community level of organization. For such assessments, assessors may use the Water Environmental Research Foundation (WERF) approach to derive a cumulative effects curve with confidence limits for the entire community of interest (see Parkhurst *et al.* 1996). This approach involves (i) calculating the effects level of interest for each species or genus (e.g., LC_{50}s, IC_{25}s), (ii) arranging the data in cumulative form for percentage of species or genera affected versus concentration, (iii) fitting a model to the effects data, and (iv) calculating confidence limits for the modelled curve. The WERF approach is described in more detail in Sections 6.3.6 and 8.6.5.5 of the resource document for single substances and complex substances, respectively.

6.3.3 *Procedure for Estimating Low Toxic Effects: Regression-Based Approach*

Step 1 Prepare a graphical summary of the concentration–response curve. This is the simplest means of showing the relationship, and, by including replicates, the degree of scatter may be examined and outliers identified. This information may then be used to choose an appropriate statistical analysis or to evaluate the scientific validity of the analysis reported by the author.

Step 2 Choose an appropriate regression model. For quantal endpoints, the probit and linear logistic models are usually appropriate choices. For quantitative endpoints, there is a wide variety of models to choose from, including the Weibull model and others that have been adapted to include control responses as a separate parameter (e.g., logistic model described in Seefeldt *et al.* 1995). U-shaped models may be required for endpoints exhibiting stimulation at low concentrations (see Downs 1992).

Step 3 Transform the independent and dependent variables as necessary to meet the assumptions of the regression analysis. Concentrations should be $\log_e$ or $\log_{10}$ transformed depending on which transformation produces the most symmetrical concentration–response curve. With quantitative data (e.g., growth rate, biomass), it is not advisable to standardize the data to controls, as this reduces the degrees of freedom available for the analysis and eliminates treatment replicates with responses greater than those of the controls. With this type of data, it is preferable to handle controls as a separate model parameter. If there is a relationship between variance and magnitude of observed responses, transformations such as the square root transformation may be required to ensure that the homogeneity of variances assumption is met.

Step 4 Perform the regression analysis using any of a variety of statistical packages (e.g., SAS, Statgraphics, SPSS, ToxCalc). An EXCEL spreadsheet package is available in the Chemicals Evaluation Division of Environment Canada (Caux and Moore 1997). The package at present includes five models (i.e., three models in the logistic family, probit, Weibull) and goodness-of-fit statistics, and it automatically calculates effects concentrations for effects ranging from 0.1 to 99.9% using nonlinear regression.

A wider range of models is available with nonlinear regression analysis. The trade-off is that the calculation of confidence limits is much more complicated. If the data can be linearized (e.g., by means of a probit or logit transformation), a weighted linear regression can be performed. With weighted linear regression, calculation of confidence limits is straightforward.

Step 5 Test model adequacy with a goodness-of-fit statistic (e.g., chi-square test or *G*-test for quantal data, *F*-test for quantitative data), and, if model fit is adequate

($p \geq 0.05$), the results can be used to derive CTVs if all other assumptions of the regression analysis are met. Regression analysis assumes that the errors are independent, have zero mean, have a constant variance, and follow a normal distribution (Draper and Smith 1981). To confirm that these assumptions have been met, the residuals from the fitted concentration-response model should be examined or formally tested.

6.3.4 Procedure for Estimating Low Toxic Effects: Hypothesis-Testing Approach

ANOVA is the most common hypothesis-testing method for estimating LOELs and NOELs. Generally, the first step is to transform the data to stabilize the variances between treatments. The transformation depends on the type of data but may include, for example, an arcsine square root transformation for response data expressed as a proportion (e.g., percentage of normal larvae at hatch) (Draper and Smith 1981; Gelber *et al.* 1985). Such a transformation is necessary because the ANOVA procedure assumes that the treatments exhibit homogeneity of variance. This assumption is routinely tested in most statistical software packages, using, for example, Bartlett's test. ANOVA also assumes that the data are normally distributed, although ANOVA is fairly robust to this assumption. If the assumptions of the ANOVA are violated, nonparametric tests such as the Shapiro-Wilks and Kruskal-Wallis tests may be used as alternatives.

The next step is to test for equivalence of the solvent carrier and noncarrier control treatments with a *t*-test. The ANOVA is then performed on the treatment groups, and, if the null hypothesis that all treatments have the same effect is rejected (i.e., a significant *F*-score, usually at $p < 0.05$), multiple comparison tests (i.e., Dunnett's procedure or preferably William's test) are performed between treatment groups to determine which treatments are different from the control treatment. The LOEL is the lowest concentration producing a significant effect in the multiple comparison tests; the NOEL is the highest concentration not producing a significant effect. The MATC is generally reported as the range between the NOEL and LOEL or as the geometric mean of the two concentrations. A variety of statistics textbooks describe ANOVA techniques, related techniques such as analysis of covariance and two-way ANOVA, and nonparametric techniques in much more detail (e.g., Snedecor and Cochran 1980; Sokal and Rohlf 1981; Zar 1984). ANOVA and related techniques are included in a wide variety of software packages, including Systat, SPSS, SAS, and Statgraphics.

6.3.5 Estimating Median Toxic Effects

From a practical point of view, rigid rules are not required for selecting among the available graphical and statistical procedures available for estimating median toxic effects. For most types of data, the estimates of the median lethal or effective concentration will not vary significantly (Stephan 1977). Commonly used methods include regression analysis (see Section 6.3.3), moving-average interpolation, and the Spearman-Karber and trimmed Spearman-Karber methods. The crucial point for assessors is to ensure that, for any given method, the assumptions have been met (e.g., normality for parametric methods) and the limitations understood (e.g., confidence limits cannot be calculated with graphical interpolation, quartiles other than 50% lethal or effective concentration cannot be calculated with moving-average interpolation). A variety of statistical packages can be used to estimate median toxic effects.

6.4 Aquatic Effects Characterization

6.4.1 Pelagic Biota[1]

The results of single-species or multispecies toxicity tests have often been used to estimate no-effects concentrations or to derive water quality objectives or guidelines for substances. For the surface water compartment, results from long-term toxicity tests

[1] Pelagic biota are free-swimming or free-floating aquatic organisms that inhabit the water column.

for organisms from different trophic levels can help determine which populations, communities, and ecosystem processes may be particularly susceptible to adverse effects and to determine the types and magnitude of these effects. From the set of acceptable studies, the test result indicating the lowest toxic effect (e.g., the lowest derived EC_{10}) should be used as the CTV for pelagic biota.

For most substances, results from single-species toxicity tests will probably be the most abundant source of effects data on pelagic biota. However, results from multispecies tests and ecoepidemiology studies can be extremely useful in characterizing direct and indirect effects under natural or near-natural conditions. Field test results are particularly valuable when characterizing the effects of complex mixtures and effluents on pelagic biota. The CBB approach is particularly relevant when it is difficult to determine the concentration of bioavailable forms of a substance in the environment (Section 6.2).

6.4.2 Benthic Biota

Sediments are an important component of aquatic ecosystems. They provide habitat to organisms — such as microorganisms, aquatic plants, annelids, insects, amphipods, and molluscs — that spend a major portion of their life cycle living on or in aquatic sediments. Sediments act as sinks and, subsequently, as sources of substances that have entered the aquatic environment. Substances found in sediments may adversely affect benthic species or bioaccumulate in benthos and subsequently be transferred to higher trophic levels.

The Water Quality Institute and RIVM (1995) provide a compendium of available standardized test methods. Environment Canada (1994, 1995) has a number of sediment toxicity guidance documents for aspects that are not covered in the standard methods and are of general application to any sediment test. Canada has produced a few standard methods applicable to sediment toxicity testing, including testing of pore water with echinoids (Environment Canada 1992a) and a solid-phase bioluminescent bacteria test (Environment Canada 1992b). Environment Canada (1992c) has also published an acute test for sediment toxicity using marine or estuarine amphipods. However, only a limited number of these spiked-sediment toxicity tests have been standardized to examine an organism's exposure to sediment-associated substances such as whole sediment, pore waters, or elutriates. Despite the paucity of standardized tests, a number of approaches have been developed to evaluate the toxicological significance of substances in freshwater, marine, and estuarine sediments. Overall, assessors should be flexible. They will need to evaluate potentially relevant benthic toxicity information by applying sound scientific principles and basic QA/QC considerations.[2] Owing to the complexities of interpreting data in the sediment compartment, assessors are advised to consult with sediment specialists when applying the following approaches.

Assessors should locate all acceptable sediment toxicological data on Canadian marine and freshwater species. Ideally, these data should cover a range of feeding behaviours, substrate preferences, locomotion, and degree of association of benthic organisms with bottom sediments. Sediment toxicity tests must use the appropriate sediment phases — such as pore water — because benthic organisms may be exposed to some or all of these phases during their life cycle. Qualitative and quantitative sources of uncertainty with the toxicological data should be documented. These uncertainties will be taken into account in selecting application factors or in conducting the uncertainty analysis during risk characterization.

Spiked-sediment toxicity tests establish cause-and-effect relationships between exposed organisms and spiked concentrations of individual substances or mixtures (Water Quality Institute and RIVM 1995). A spiked-sediment toxicity test is directly analogous to a water column test, except the substance and test species are added to solid-phase sediments. Researchers can use sediment

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2 See Important Considerations in Section 6.4.2 and Appendix III, respectively, of the resource document.

from a reference location to provide interlaboratory comparability. Artificially prepared sediments may also be used instead of field sediments, thereby avoiding concerns that the sediments may have been contaminated with other substances. Assessors should be aware of concerns regarding the viability of organisms in artificial sediments. Data interpretation still relies on expert judgment. For example, sediment spiking may be strongly influenced by the methodology, and this may affect the comparability of results.

As with pelagic biota, single-species toxicity tests may be used to determine CTVs for sediment-dwelling biota. Toxicity tests may be short-term acute or longer-term chronic.

A weight-of-evidence approach can be used to establish associations between a substance's concentration in sediments and observed adverse biological effects. For example, the EqP approach provides a link to effects on benthic organisms. These associations can be based on data from laboratory tests conducted on field-collected sediments that contain mixtures of substances. These are referred to as co-occurrence data. Field data in the literature should be evaluated on a case-by-case basis to determine their usefulness. Co-occurrence data are often site-specific. Caution must be used in extrapolating results to other sites.

CCME (1995) provides a discussion of the co-occurrence approach based on work by Long and Morgan (1990), Long (1992), and Long and MacDonald (1992). Other types of co-occurrence approaches include the apparent effects threshold (AET), sediment quality triad, and informal evaluations of chemistry and biological responses (U.S. EPA 1992c). Sediment specialists will be identified for risk assessors to consult when applying a co-occurrence approach.

The benthic community structure assessment is another weight-of-evidence approach that may be used to compare a community living at a reference station with a community living in a contaminated area. This allows assessors to determine whether effects have occurred on infaunal species and to identify spatial and temporal trends in sediment contamination.[3] For example, this information can be used to determine if a mixture of substances has affected community dynamics downstream of an industry. This weight-of-evidence approach is a recognized *in situ* method for determining sediment quality. It can be applied to a wide variety of aquatic ecosystems and to a wide variety of chemical groups. However, this approach does not identify substances found in the mixture.

The EqP approach (Section 6.2.7) may be used for organic substances when the sediment solid phase contains more than 0.2% organic carbon (Di Toro *et al.* 1991). An analogous approach has been proposed for cationic metals (Campbell and Tessier 1996). A key parameter, for both organic contaminants and metals, is the free solute concentration in the sediment pore water. This is true not because pore water is necessarily an important medium for uptake, but rather because $[\text{solute}]_{\text{free}}$ is a good estimate of the solute's chemical activity and overall bioavailability in the sediment matrix. The EqP approach yields estimates of this key parameter (Di Toro *et al.* 1991; Campbell and Tessier 1996).

Sediment quality guidelines and standards from various jurisdictions should also be reviewed for possible information on priority substances (e.g., CCME 1995).

6.4.3 Groundwater Biota

Groundwater occupies pores and crevices in rock and soil in the phreatic or saturated zone. Traditionally, it has been a resource for drinking water, agriculture, and industry. However, recent investigations have shown that a biologically diverse ecosystem exists within groundwater. The groundwater ecosystem provides habitat, food, and nutrients for microbes such as bacteria and protozoa (Chapelle 1993) and for micro- and macroinvertebrates, especially crustaceans (Botosaneanu 1986; Danielopol 1992;

[3] Examples of this approach are given by Diaz (1992), La Point and Fairchild (1992), Persaud *et al.* (1992), Reynoldson and Zarull (1993), and Reynoldson *et al.* (1995).

Marmonier *et al.* 1993). Biochemical reactions (aerobic and anaerobic respiration, fermentation, etc.) performed by bacteria in the subsurface influence the chemical composition of groundwater. Protozoa and multicellular organisms operate more indirectly on water quality because of their influence on bacterial biomass, growth, and metabolic state. Also, the self-cleansing potential of aquifers is related to these processes (Chapelle 1993; Stanford and Vallett 1994). There is now more research into groundwater ecosystem dynamics and function, the identification and distribution of groundwater organisms, and the effects of contaminants on groundwater organisms.

While there are many approaches to evaluate the effects of priority substances in surface water, research to determine the effects of substances on natural populations of groundwater ecosystems is an emerging field. No standard toxicity test protocols exist for groundwater organisms, and only effects on bacterial mineralization rates[4] (Van Beelen *et al.* 1991) and acute toxicity tests with groundwater invertebrates are described in the literature (Notenboom *et al.* 1994). Assessors should use all available data as long as good general QA/QC practices and sound scientific principles are followed. In addition, all available data from the approaches described below should be included in a weight-of-evidence approach. Owing to the difficulty in interpreting effects data for groundwater and surrogate organisms, assessors are advised to consult with groundwater ecology experts.

Substances with low K_{ow} and K_{oc} values are of the most concern to groundwater biota, because they travel the furthest distance and may create the largest plume (Lesage 1995). However, substances with a high K_{ow} may also be of concern by desorbing slowly from organic matter to which they had adsorbed in the saturated zone. The organic matter may then be a source of contamination of substances for a long time. High K_{oc} and K_{ow} values also favour substance transport on colloids (Lafrance *et al.* 1989; McCarthy and Zachara 1989; Kan and Tomson 1990).

Leaching potential is also affected by a substance's transformation rate in the soil (Boesten and van der Linden 1991). Generally, owing to the low organic matter content of aquifers, there is low sorption capacity and, consequently, relatively high bioavailability. Groundwater invertebrates generally require some measurable dissolved oxygen and therefore a more positive redox potential. These parameters can be good diagnostic variables (although sometimes difficult to measure easily in these habitats). The assessor should be aware of the physical and chemical properties of the substance and the material through which it is being transported.

Simple exposure screening strategies and laboratory toxicity tests are recommended for evaluating effects on groundwater organisms. Test organisms should be representative of Canadian species and of groundwater biota in terms of function, trophic level, and route of exposure. When reviewing toxicity studies, assessors should be aware of the influence of pH, oxygen content, temperature, and other parameters on the bioavailability of organic and inorganic substances and hence on their toxicity. For more discussion, see Important Considerations in Section 6.4.3 of the resource document.

In practice, groundwater toxicity data will probably be unavailable. If, however, groundwater biota have been identified as being exposed to elevated levels of a substance, surrogate species such as surface water crustaceans may be used to determine the CTV for functionally similar species (Notenboom *et al.* 1994). Other candidates for surrogate species can be found among rotifers, nematodes, protozoans, and oligochaetes. These taxa, in addition to crustaceans, are frequently found in groundwater and are also used in ecotoxicology studies. It is also possible that effects threshold data for groundwater organisms could be estimated from toxicity results from soil-dwelling organisms such as earthworms (van den Berg and Roels 1991). For Tier 1 assessments, toxicity data from surrogate species (aquatic crustaceans, protozoans, nematodes, and oligochaetes) can be used. Again, assessors are advised to consult with groundwater ecology experts when approaching this type of assessment.

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4 This refers to the measurement of the ability of the bacteria to mineralize a given substrate/substance.

Assessors should identify areas of qualitative and quantitative uncertainty in the toxicological data. These may include uncertainties regarding the relationship between the substance and the groundwater ecosystem, the parameters of the study, and natural variations in groundwater systems. When using toxicity data measured for aquatic surface water species to derive, extrapolate, or otherwise estimate toxicity data for species in groundwater, it is important that the uncertainty be characterized.

The CTV is obtained from a weight-of-evidence approach that examines all appropriate data. Chronic, full life cycle studies measuring nonlethal effects such as growth and reproduction are preferred. The EqP method (Section 6.2.7) may also contribute to the weight-of-evidence approach. If only acute toxicity data are available or if the acute toxicity data are more sensitive than the chronic information, the CTV may be based on an LC_{50}, EC_{50}, or other significant EC_x.

6.5 Terrestrial Effects Characterization

6.5.1 Soil Biota

Substances found in soils may exist as distinct solid or liquid phases or may be dissolved in the soil water, vaporized in the soil air, or adsorbed or absorbed to mineral or organic particles. Soil properties play a key role in determining the bioavailability of a substance to soil organisms. These properties include soil particle size distribution (percentage of sand, silt, and clay), moisture content, pH, total organic carbon content, and redox potential (Section 5.3 in the resource document).

For assessment purposes, soil biota are organisms that live at least part of their life cycle in the soil. They may live above ground, in the litter layer, in the mineral soil, or in soil pore water. Soil biota include microorganisms, fungi, invertebrates, and plants. Mammals, birds, reptiles, and amphibians are assessed separately as wildlife (see below).

There are a variety of approaches to assess the effects of priority substances on soil-dwelling biota, including single-species and multispecies toxicity tests and field studies. Toxicity test protocols have been developed to assess effects on earthworms and terrestrial plants (U.S. EPA 1985; OECD 1993a). However, the only internationally harmonized soil toxicity test using invertebrates is the acute earthworm toxicity test (OECD 1984). See Section 6.6.1 in the resource document for a description of this test and other tests currently undergoing research to standardize lethal and sublethal toxicity tests for a wider range of soil-dwelling organisms.

Data should be evaluated based on good general QA/QC practices and sound scientific principles (see Appendix III in the resource document; Environment Canada 1996). Toxicity information should ideally include data from a wide range of trophic levels and from both above ground and soil-dwelling biota. Soil organisms can be exposed to substances in soil via three routes: (i) oral uptake of food, soil particles, or pore water, (ii) dermal uptake from contact with pore water or soil particles, and (iii) inhalation of soil air (see Table 5.6 of the resource document). Assessors should therefore consider the partitioning of the substance within soil compartments and the life habits of the soil biota to determine the relevance of toxicity test data. Toxicity studies considered in assessments should use test organisms and soil with properties that are representative of the areas of concern in the Canadian environment.

Toxicity information should include data from important trophic levels and functions such as decomposition (microorganisms and detritivores), primary production (plants), and herbivores and saprovores (invertebrate fauna). To compare these tests, standardized soil that has similar textural composition, pH, organic matter content, water content, and density should be used (van Leeuven and Hermens 1995).

Acute and chronic toxicity data for aquatic species may be used as a screening tool to estimate effects on soil organisms that are exposed primarily to a substance via soil pore water. Aquatic species that can be used as surrogates for related terrestrial organisms include crustaceans, insect larvae, annelids, plants, and algae (VKI 1994). Two modifying factors must be considered — namely, soil organic carbon content (f_{oc}) and soil water content (f_w), such that:

$$CTV_s = [(f_{oc} \bullet K_{oc}) + f_w] \bullet CTV_d$$

where

CTV_s	=	CTV for soil biota
f_{oc}	=	mass fraction of organic carbon in the solid phase
K_{oc}	=	organic carbon partitioning coefficient (where $K_{oc} \approx K_{ow}$, the octanol–water partition coefficient)
f_w	=	mass fraction of water content in soil
CTV_d	=	CTV of the dissolved substance on an aquatic organism (modified from VKI 1994).

Predictive approaches, such as the EqP approach and QSARs, can provide supporting information as part of the weight-of-evidence determination but should not be used alone to derive the CTV. These approaches involve considerable uncertainty. Assessors should consult Sections 6.2.6 and 6.2.5, respectively, of the resource document for information on the EqP method and QSARs.

Soil quality guidelines and standards from various jurisdictions should also be reviewed for possible information on priority substances (e.g., CCME 1996).

6.5.2 Wildlife

For assessment purposes, wildlife refers to wild mammals, birds, amphibians, and reptiles. Because of the complexities in predicting the effects of substances on wildlife, assessors should consult with the Canadian Wildlife Service when parameters related to wildlife are the assessment endpoints.

Wildlife may be exposed to substances through inhalation; dermal contact with soil, sediment, water, or air; oral intake of aquatic or terrestrial prey and water; incidental ingestion of soil or sediment; or cleaning feathers or fur. Assessment and measurement endpoints should involve similar exposure routes. For a volatile substance that partitions to the air, an inhalation study is preferred. For a hydrophobic substance that partitions to biota, an oral ingestion study is preferred. The Canadian Wildlife Service is developing a computerized Wildlife Contaminant Exposure Model (WCEM) to estimate wildlife exposure to organic substances through inhalation and ingestion of food and water in the Canadian environment (Brownlee *et al.* 1995). All of the major routes of substance exposure identified in this model should be assessed.

Wildlife-testing protocols have been reviewed recently by Hoffman *et al.* (1995). Avian protocols include acute oral (LC_{50}), short-term dietary (LD_{50}), chronic reproduction, embryo toxicity/ teratogenicity, behavioural, and field toxicity tests. Mammalian wildlife assessments rely heavily on laboratory data (Hodgson and Levi 1987) generated for human assessments, although U.S. EPA protocols are available for the mink (*Mustela vison*) and European ferret (*Mustela putorius furo*) (Ringer *et al.* 1991). A standardized frog embryo teratogenesis assay (FETAX) has been developed by ASTM (1991). There are no terrestrial toxicity test protocols for amphibians. However, the aquatic life stages appear to be the most sensitive to potentially harmful substances.

The range of sensitivity to environmental substances depends on taxonomic class, age, size, and life history characteristics. For example, birds are generally considered more sensitive than mammals, amphibians, or reptiles. Smaller species consume more substance per unit body weight. These generalizations should be applied with caution, as there are always exceptions (Tucker and Leitzke 1979). Owing to differences in wildlife physiology and sensitivity between classes, interclass extrapolations of quantitative data are not recommended. However, when physiological similarities between classes and the mechanism of action are known, data may be discussed qualitatively in relation to another class to provide supporting evidence for the assessment.

For wildlife, measurement endpoints such as reproductive and developmental toxicity[5] and reduced survival are preferred, as they can be directly related to potential population-level effects. A substance may also have an impact on wildlife populations through behavioural alterations, decreased food supply, or habitat degradation. Chronic studies on organ-specific effects may be used if the effect can potentially reduce survival or reproduction in wildlife. Biochemical or physiological perturbations such as endocrine disruption, genotoxicity, and immune suppression may also have serious repercussions for wildlife population effects. However, there are no standard measurement endpoints for identifying population-level effects for some of these examples.

Field studies are preferred when cause-and-effect relationships can be clearly established to derive a CTV for wildlife. They can integrate many environmental factors that cannot be replicated in a laboratory study. When field studies are unavailable, laboratory studies may be used, with preference given to wildlife species. CBB studies (Section 6.2.5) and other body burden studies may also be relevant, particularly for metals.

6.6 Effects Mediated Through the Atmosphere

Substances identified during problem formulation that are likely to partition to the atmosphere may be assessed under either Section 11(a) or Section 11(b) of CEPA. Their behaviour should be compared with that of substances known to cause stratospheric ozone depletion, ground-level ozone formation, or global warming using one or more of the methods outlined below. These methods provide a rough estimate for the potentials described, and, although they can be calculated quickly, their real value may be for screening during problem formulation and as indicators for more in-depth study.

Under Section 11(b), "toxic" determinations will include effects due to stratospheric ozone depletion and ground-level ozone formation.

Global warming resulting from climate change is assessed under Section 11(a) of CEPA, as it is considered to cause direct adverse effects on the environment or because there is no clearly defined link to specific human health effects. "Toxic" determinations for all atmospheric effects may not be straightforward because of the complexities in predicting potential atmospheric interactions. However, assessors should consult with experts in the Atmospheric Environment Service of Environment Canada or elsewhere for assistance.

The following sections summarize the methods available for estimating a first approximation of the various potentials of atmospheric effects.

6.6.1 Stratospheric Ozone Depletion

Ozone-depleting potential (ODP) is the ratio of calculated ozone column change for each mass unit of a gas emitted into the atmosphere relative to the depletion calculated for an equal mass of reference gas, chlorofluorocarbon-11 (CFC-11) (ODP = 1). An example of a calculation is provided in Section 6.6.3 of the resource document. In a first approximation, the ODP value can be calculated using the formula:

$$ODP = (T_S/T_{CFC\text{-}11})\,(M_{CFC\text{-}11}/M_S)\,([n_{Cl} + \alpha n_{Br}]/3)$$

where

T_S	=	atmospheric lifetime of substance S (years)
$T_{CFC\text{-}11}$	=	atmospheric lifetime of CFC-11 (60 years)
$M_{CFC\text{-}11}$	=	molecular mass of CFC-11 ($137.5 g \bullet mol^{-1}$)
M_S	=	molecular mass of substance S ($g \bullet mol^{-1}$)
n_{Cl}	=	number of Cl atoms per molecule
n_{Br}	=	number of Br atoms per molecule
α	=	a measure of the effectiveness of Br in ozone depletion with respect to Cl; a reasonable parameter is $\alpha = 30$.

[5] Includes effects on spermatogenesis, fertility, pregnancy rate, number of live embryos, neonatal mortality, eggshell thinning, egg production, hatchability, and offspring survival.

In general, ODP values approach zero for species with atmospheric lifetimes less than one year. In accord with the Montreal Protocol on Ozone Depleting Substances, any substance with an ODP may be considered "toxic" under Section 11(b) of CEPA and subject to regulation.

6.6.2 Ground-Level Ozone Formation

Substances that contribute to ground-level ozone formation are volatile, reactive hydrocarbon gases (volatile organic compounds, or VOCs) at ambient tropospheric temperatures. Such substances possess a wide range of ozone-producing potentials.

The photochemical ozone creation potential (POCP) index measures the relative effect on ozone of a unit mass of any organic compound compared with that of an equivalent mass of ethene (CEU 1995). Ethene has a POCP value of 100. A first indication of episodic ozone formation can be obtained from a reactivity scale based on the rate constant for the reaction of substance S with hydroxyl radicals and the molecular weight of substance S compared with that of ethene. An example of the calculation is shown in Section 6.6.3 of the resource document using the equation below:

$$\text{OH-scale} = (k_S/M_S)\,(M_{ethene}/k_{ethene}) \times 100$$

where

k = rate constant at T = 298 K for the reaction with hydroxyl radicals ($cm^3 \bullet mol^{-1} \bullet s^{-1}$)

k_S = rate constant for the reaction of substance S with hydroxyl radicals ($cm^3 \bullet mol^{-1} \bullet s^{-1}$)

k_{ethene} = rate constant for the reaction of ethene with hydroxyl radicals ($8.5 \times 10^{-12}\ cm^3 \bullet mol^{-1} \bullet s^{-1}$)

M_S = molecular mass of substance S ($g \bullet mol^{-1}$)

M_{ethene} = molecular mass of ethene ($28\ g \bullet mol^{-1}$).

There is too much uncertainty associated with this methodology to assign an ozone-forming potential (OFP) threshold above which a VOC could be considered "toxic" under CEPA Section 11(b). However, with technical assistance, it may be possible to generate more accurate OFPs.

Computer simulations can be used by appropriate experts to arrive at more precise estimates of the ozone creation potential for individual organic compounds (Carter 1994). These simulations produce reactivity scales that take into account kinetic and mechanistic reactivity. In general, reactivity scales numerically rank each VOC, providing a measure of how its emissions affect ozone formation.

Two sets of reactivity factors have been calculated: the maximum incremental reactivity (MIR) scale and the maximum ozone incremental reactivity (MOIR) scale. Many substances already have published values for their reactivity, or these values can be generated, if necessary (Dann 1994).

With more precision, it may be easier to determine the extent of the contribution of any given VOC to ground-level ozone formation. However, the problem of defining a threshold for that contribution to be "toxic" under CEPA Section 11(b) remains.

Consequently, until a consensus is reached about what constitutes a "toxic" determination under CEPA Section 11(b) for ground-level ozone formation and about the magnitude of the associated threshold, evidence of ozone formation should be used only in combination with other data, such as direct effects on biota or human health.

6.6.3 Global Warming

Global warming potential (GWP) is the ratio of warming for each unit mass of a gas emitted into the atmosphere relative to the warming for a mass unit of the reference gas CFC-11. Assessors will be able to estimate the GWP of a substance S using the following formula. An example of a calculation is given in Section 6.6.3 of the resource document using the equation below:

$$GWP = (T_S/T_{CFC\text{-}11})\ (M_{CFC\text{-}11}/M_S)\ (S_S/S_{CFC\text{-}11})$$

where

T_S = atmospheric lifetime of substance S (years)

$T_{CFC\text{-}11}$ = atmospheric lifetime of CFC-11 (60 years)

M_S = molecular mass of substance S ($g \bullet mol^{-1}$)

$M_{CFC\text{-}11}$ = molecular mass of CFC-11 (137.5 $g \bullet mol^{-1}$)

S_S = IR absorption strength of substance S in the interval 800–1200 cm^{-1} ($cm^{-2} \bullet atm^{-1}$)

$S_{CFC\text{-}11}$ = IR absorption strength of CFC-11 in the interval 800–1200 cm^{-1} (2389 $cm^{-2} \bullet atm^{-1}$).

Methods for deriving absorption strengths (S_S) are described by Kagann *et al.* (1983), Rogers and Stephens (1988), and CEU (1995). Using this calculation, substances with an estimated GWP of 0.05 or greater would be a concern.

GWP estimates are useful in developing a weight-of-evidence approach under Section 11(a) of CEPA for assessing trace gases that could disrupt the radiative balance of the Earth. Further consultations will be necessary to derive "toxic" thresholds under Section 11(a) of CEPA for these substances.

6.7 Some Points to Remember

- Present all relevant data sets and models pertaining to potential effects on assessment and measurement endpoints.
- For dose–response curves, include both upper and lower confidence limits and some measure of central tendency.
- Indicate how dose–response relationships change with alternative data sets, assumptions, and models.
- Give a rationale for preferred data sets and models used in the effects characterization. Discuss the strengths and weaknesses of preferred data sets, and indicate the scientific consensus or lack thereof for critical issues or assumptions.

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CHAPTER 7

RISK CHARACTERIZATION

7.1 Introduction

7.1.1 Goals and Objectives

The objective of risk characterization is to determine the likelihood and magnitude of adverse effects on assessment endpoints as a result of exposure to the priority substance (definition adapted from Suter 1993). To do this, ecological risk assessment techniques and tools are used when appropriate and when sufficient data are available. This chapter describes a tiered approach for estimating risks of adverse effects of priority substances on assessment endpoints.

7.1.2 Relationship with Other Phases

Risk characterization combines the results of the characterization of entry, exposure, and effects (Figure 7.1). These results may be combined in a number of ways. The most common approach is to estimate exposure based on monitoring studies and toxicity based on laboratory bioassays and then compare the two. Other information should also be used in a weight-of-evidence approach whenever possible. For example, if field observations indicate a correlation between the absence of sensitive species and levels of the priority substance, this evidence should be used in characterizing risk. Similarly, if several toxicity studies or QSARs corroborate the CTV (see Chapter 6) or if fate model predictions support the monitoring data, these lines of evidence should be highlighted in the risk characterization. The use of several lines of evidence can strengthen our confidence in the risk assessment conclusions. Conversely, if the lines of evidence contradict one another, then our confidence in the risk assessment conclusions will decrease. Assessors must then try to resolve the difference by reexamining each line of evidence and, if necessary, generating new data.

7.2 Overview

A tiered approach is used for environmental assessments of priority substances under CEPA. In Tiers 1 and 2, a quotient is calculated for each assessment endpoint by dividing a single EEV by an ENEV. An ENEV is calculated by dividing the CTV by an appropriate application factor. Application factors are used to account for the uncertainties inherent in extrapolating between measurement and assessment endpoints. A Tier 1 assessment involves the calculation of deliberately hyperconservative quotients (Section 7.3). If such hyperconservative quotients are <1 for an assessment endpoint, then the likelihood that the substance is causing adverse effects in the Canadian environment is very small, and the assessment for that endpoint would not lead to the conclusion that the substance is "toxic" as defined in CEPA. For an assessment endpoint with a Tier 1 quotient ≥ 1, a more refined Tier 2 assessment is normally required. Section 7.4 describes ways of refining Tier 1 quotients to be less conservative. For an assessment endpoint with a Tier 2 quotient ≥ 1, a Tier 3 assessment should be undertaken. Tier 3 assessments are probabilistic, integrating distributions of exposure and/or effects. This approach facilitates a more explicit consideration of sources of variability and uncertainty in the risk analysis. This analysis considers not only the risk of exceeding the ENEV, but also the entire relationship between exposure and response, in order to estimate the probabilities of effects of differing magnitudes.

Ecological risk assessment techniques are particularly well suited for Tier 3 assessments. Section 7.5 describes the procedures for a Tier 3 probabilistic risk analysis.

For many naturally occurring substances, there are naturally enriched areas in Canada. In these areas, resident organisms will have developed a tolerance to the substance of interest. However, there is a potential for harmful effects to these resident organisms if exposure is further increased as a result of anthropogenic sources. Assessments of naturally occurring substances therefore involve estimating background concentrations and adjusting ENEVs to account for expected tolerances in naturally enriched areas. This is discussed in Section 7.6.

Risk analyses are usually based on assessment endpoints at the population or community level of organization. Assessment endpoints at the individual level may be appropriate for threatened or endangered species, where population sizes are already reduced. The quantitative prediction of mid- to long-term effects at higher levels of organization generally requires linking toxicity test results with population- or community-level simulation models or field studies. Section 7.7 provides guidance on how models and field studies may be used to quantitatively estimate the consequences of exposure to priority substances at higher levels of organization. Models and field studies may not be required for qualitative descriptions of potential consequences at higher levels of organization.

In carrying out a risk analysis at any tier, key sources of uncertainty must be identified and described either qualitatively or quantitatively. Smith and Shugart (1994) examined uncertainty in relation to the three phases of ecological risk assessment — problem formulation, analysis, and risk characterization. Uncertainties in problem formulation include choice of appropriate endpoints, models, and scale. In the analysis and risk characterization phases, potential sources of uncertainty include:

- incomplete knowledge of the composition, magnitude, frequency, and duration of releases and discharges,
- incomplete knowledge of the physical and chemical properties of the substance,
- incomplete understanding of the temporal and spatial scales of exposure and the matching of those scales with the ecological scales of the risk assessment,
- incomplete knowledge of substance transformation due to chemical, physical, and biological actions,
- poor understanding of the heterogeneity of the populations at risk,
- incomplete knowledge of how stressors act upon a population or community and the interactions among multiple stressors,
- inadequate reproducibility of laboratory and field studies,
- incomplete knowledge of the extrapolation of laboratory toxicity test results to field conditions, and
- incomplete knowledge of the extrapolation of toxicity test results for measurement endpoints to assessment endpoints.

In deciding whether these or other sources of uncertainty are critical to the assessment of whether or not a substance is CEPA "toxic" or for effective risk management decisions, assessors should communicate regularly with Environment Canada risk managers and interested parties throughout the risk characterization phase. Assessors, managers, and interested parties will need to consider which analyses will ultimately be the most useful during risk management. They will also need to decide when the analyses have proceeded far enough. Regular communications with risk managers and interested parties will help to ensure that the risk assessment plays a central role whenever it is necessary to develop strategic options for priority substances.

7.3 Tier 1: Hyperconservative Quotients

Tier 1 of an environmental assessment involves calculating a hyperconservative quotient (i.e., EEV/ENEV) for each assessment endpoint. For a Tier 1 quotient, the EEV is usually the maximum total observed or predicted concentration or dose in the environment, and the application factor used in

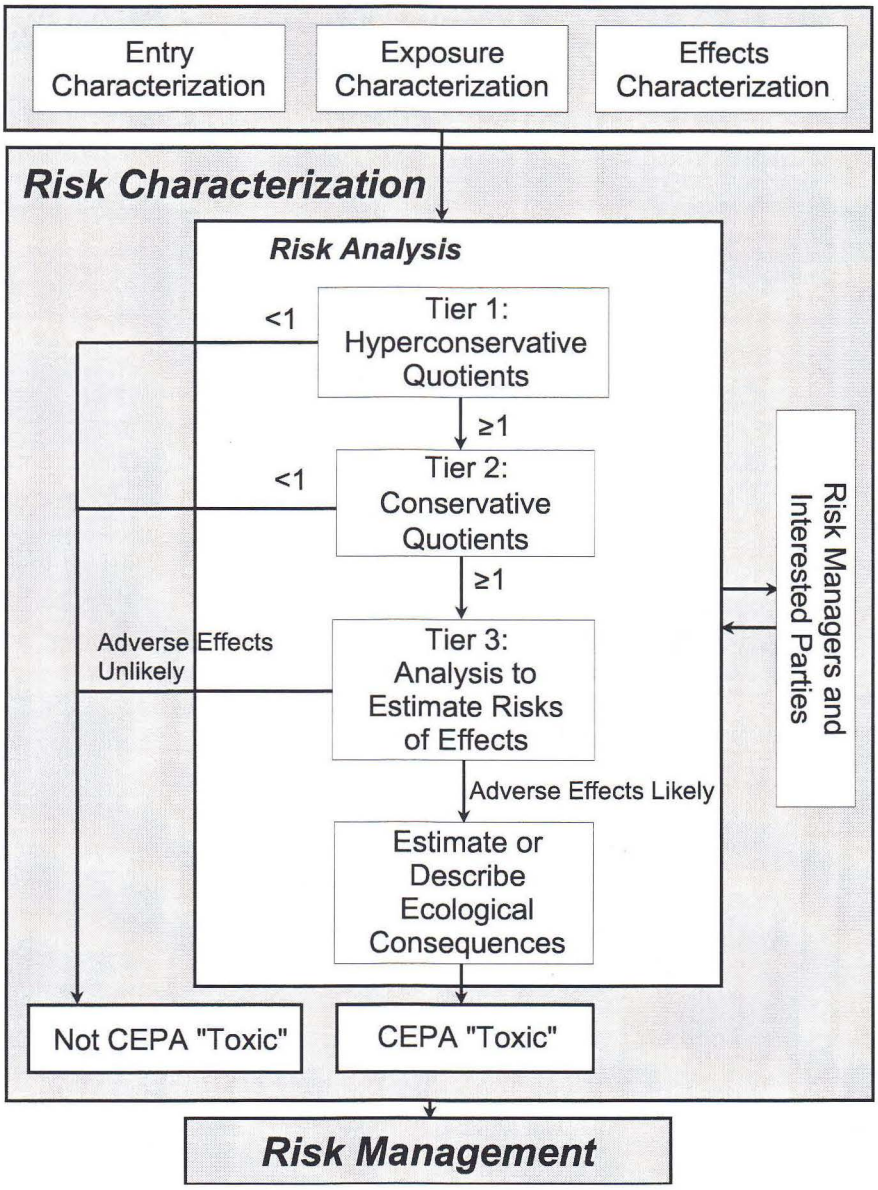

Figure 7.1 Risk characterization in the ecological risk assessment framework for priority substances.

deriving the ENEV may be large. The recommended maximum application factors presented in Table 7.1 are similar to those used by a number of other agencies (Environment Canada 1996). Typically, hyperconservative scenarios overestimate the risk posed to assessment endpoints (Bogen 1994; Cullen 1994). If the hyperconservative quotient is <1 for an assessment endpoint, there is a very low probability of adverse effects on the assessment endpoint, and there is little justification in proceeding to more detailed analyses. The substance is not declared "toxic" as defined in Section 11 of CEPA, based on the assessment of that endpoint. For an assessment endpoint with a hyperconservative quotient ≥1, the assessment proceeds to a less conservative, more realistic Tier 2 analysis.

Table 7.1 Recommended maximum application factors for converting critical toxicity values to estimated no-effects values in Tier 1.

Available Information	Maximum Factor
Threshold (e.g., IC_{25}) of sublethal toxicity from a base data set (e.g., fish, daphnid, and algal species)	10
Lowest acute LC_{50} or EC_{50} from a base data set (e.g., fish, daphnid, and algal species)	100
Lowest acute LC_{50} or EC_{50} from a data set of one or two species	1000

7.4 Tier 2: Conservative Quotients

A Tier 2 environmental assessment of a priority substance involves a further analysis of exposure and/or effects to calculate a quotient that is still conservative, but more "realistic" than the hyperconservative quotient calculated in Tier 1. For example, the EEV should be based on more recent data and on the bioavailable fraction, rather than on total concentrations. When possible, the CTV should be derived from studies using test organisms that are closely related to species resident in areas of concern, rather than from results of studies using the most sensitive species, if they are not related to the assessment endpoint. It may be possible to decrease the size of the application factor used to derive the ENEV from the CTV (from, for example, 100 to 20) if the substance is nonpersistent and does not bioaccumulate or if QSAR or EqP calculations support the CTV. When available, empirically derived acute/chronic ratios (ACRs) should be used to estimate long-term no-effects concentrations from the results of acute toxicity studies (Kenaga 1982). It may be necessary to carry out research to generate exposure and/or effects data in order to complete Tier 2. If the Tier 2 quotients are <1 for an assessment endpoint, there is a low probability of adverse effects, and the substance is not declared "toxic" on the basis of that assessment endpoint. For quotients ≥ 1, assessments should proceed to Tier 3 to estimate the potential risks posed by the substance.

7.5 Tier 3 Analyses

Tier 3 analyses consider distributions of exposure and/or effects. This approach allows a more thorough consideration of sources of variability and uncertainty in the risk analysis. These distributions can be analyzed, and the results of the analyses presented, in a variety of ways. The following guidance is provisional and will be updated when further experience is gained in applying Tier 3 methods to priority substances.

In its simplest form, Tier 3 assesses the risk or probability of exceeding the ENEV by comparing the exposure distribution with the point estimate ENEV. Tier 3 may be more complex, using ecological risk assessment techniques and tools to compare distributions of both exposure and effects in order to estimate the probabilities of differing magnitudes of effects. Assessors should consult with risk managers to determine the appropriate approach.

Choosing appropriate models and methods of analyses for a Tier 3 assessment is more involved and difficult than in Tiers 1 and 2. The methods used to estimate risks should be capable of propagating variabilities and uncertainties through the analysis and, if possible, estimating ecological consequences. This requires more emphasis on site characteristics to estimate exposure and on the sensitivities of resident biota to characterize effects.

Tier 3 estimates of risk may be obtained by a variety methods, including first-order error analysis, Monte Carlo simulation, Baye's method, and others. These methods produce a single number that estimates the probability of a specified effect or a distribution of output that provides information on the probabilities of a range of effects (Covello and Merkhofer 1993; Smith and Shugart 1994). The method selected by the assessor will depend on the nature of the problem and the available information. For substances for which the determination of "toxic" is not clear-cut, it is impossible to specify universal probability cutoffs that are sufficient for a "toxic" determination, as issues of magnitude of effects, spatial and temporal scales of effects, and availability of supporting lines of evidence all play a role in the decision. Professional judgment is required, and the assumptions underlying the judgment must be clearly stated. Key concepts, model selection issues, and methods that assessors may use to conduct a probabilistic risk analysis are discussed below.

7.5.1 Key Concepts

The concept of probability can be difficult, because there is no universally agreed-upon definition (Power *et al.* 1994). When empirical data are plentiful and relevant to the variable of interest, development of a probability estimate can proceed using standard statistical techniques (Taylor 1993). For example, substance concentration in sediment over a defined spatial area has a true mean, variance, and shape of distribution. If a well-designed sampling and analytical strategy has been employed, then it is possible to estimate values for the mean and variance and the shape of the distribution that are close to the true values and distribution shape. In this case, the estimated variance of substance X concentration could be used to state, for example, that a sedentary benthic organism has a 95% probability of being exposed to substance X in the concentration range 1.5–9.9 $\mu g \bullet L^{-1}$. Hoffman and Hammonds (1994) refer to this type of statement as Type A uncertainty. That is, the distribution of possible exposures for organisms is known, but the actual exposure to specific individuals is unknown. Type A uncertainty is akin to the objective or classical view of probability, in that the probability estimate is a well-defined, measurable number.

Uncertainty about a variable that is fixed or deterministic is referred to as Type B uncertainty (Hoffman and Hammonds 1994). If, for example, we had only a limited number of sediment samples in the case above, then there would be much uncertainty concerning the values for the true mean and variance and the shape of the distribution. Type B uncertainty comprises several sources of uncertainty, including (i) *model uncertainty*, resulting from lack of understanding of the ecosystem or failure to capture the salient features of risk, (ii) *parameter uncertainty*, owing to the imprecise estimates of model parameters made from limited data, (iii) *judgmental uncertainty*, arising from the inability of experts to specify precise values for model inputs when data are lacking, and (iv) *completeness uncertainty*, resulting from the possible omission of important processes from the analysis (Covello and Merkhofer 1993).

Probability estimates often include both Type A and Type B sources of uncertainty. It may be possible to separate Type A and Type B sources of uncertainty in some probabilistic risk analyses (see Hoffman and Hammonds 1994 for an example). The results of such an analysis can be thought of as a risk function with confidence limits. In practice, apportioning Type A and Type B sources of uncertainty for individual inputs is difficult.

7.5.2 General Mechanics of a Probabilistic Risk Analysis

Finkel (1990), Hammonds *et al.* (1994), and others have developed guidelines for quantifying uncertainty that include the following steps. Some of these steps are expanded upon in subsequent sections.

- Identify the desired numerical expression and characteristic of risk for each assessment endpoint (e.g., 25% mortality to pelagic fish species, 10% growth rate impairment in diving ducks) (see resource document, Section 3.1). The remaining steps need to be followed separately for each measurement and/or assessment endpoint.

- Specify the model equation that will estimate risk (Section 7.5.3).

- List all variables that will be specified as distributions. In general, it is preferable to keep this list as short as possible by specifying input distributions only for those variables that are likely to have an important influence on the output (Seiler and Alvarez 1996).

- Generate a distribution for each input variable in the risk equation (Section 7.5.4). These are often referred to as probability density functions or PDFs.

- Determine and account for dependencies among input variables. An example of a dependency would be a positive correlation between concentrations in water and concentrations in prey species in a probabilistic analysis of exposure for a predatory fish species.

- Generate the output variable distribution by combining the uncertainty distributions of the input variables as specified in the risk equation. This step often involves Monte Carlo simulation, but there are a variety of other possible methods (Section 7.5.5).

- Fine-tune the analysis. At this point, assessors may use the results of a sensitivity analysis to determine those input variables that had an important influence on the output variable. Such input variables should be reexamined to ensure that the data and distributions are scientifically acceptable. Often the tails of the input variable distributions need to be truncated to eliminate physically or logically impossible values. Input distributions may also have to be adjusted to account for dependencies between important variables. Once the input distributions and, if necessary, the model equation have been fine-tuned, the analysis is repeated and a refined output generated. Fine-tuning the risk analysis often involves numerous iterations.

- Summarize the results, highlighting important implications for risk managers. The major output of the analysis is a quantitative or graphical description of the probability of an effect (see Appendix V of the resource document for an example). Such outputs may be summarized as PDFs, cumulative probability distributions, ranges and box plots, pie charts, histograms, summary statistics, or risk indices. The objective is to ensure that the risk manager understands the results of the analysis and the impact of any uncertainties not captured in the analysis on the conclusions of the risk assessment and subsequent risk management decisions. The manager should also be informed of any unresolved scientific controversies (Finkel 1990; Covello and Merkhofer 1993).

7.5.3 Choosing an Appropriate Model

As one of the objectives of a Tier 3 assessment is to estimate probabilities of effects, in addition to simply identifying possible risks, models are required to account for spatial and temporal variation in substance concentrations and bioavailability, characteristics of the receiving environment, indirect effects, etc. The consequences of selecting one model over another should be analyzed (Smith and Shugart 1994). Assessors should consider issues such as availability of data, the appropriate aggregation level for model inputs, spatial and temporal scaling, initial condition sensitivity, applicability to the system of interest, and whether the model has been appropriately calibrated and validated, in order to minimize uncertainty about the resulting risk estimates (Beck 1987; Oreskes *et al.* 1994).

It is useful to break the process of choosing a model into two steps: model identification and model selection. In the first step, the assessor identifies those aspects of the substance and receiving environment that must be included in the model (i.e., a conceptual model is constructed). In the second step, the assessor chooses an existing analytical or computer model that expresses the conceptual model. Before proceeding with a model simulation, credibility of the model should be assessed (Suter 1993). The assessment of credibility is different from model calibration and validation, because it does not yet consider the fully parameterized form of the model. The goal is to develop a qualitative measure of the predictive accuracy of the model. The following are indications that the model of interest is credible: experimental testing on other systems (e.g., mesocosms) indicates that the model performs adequately, the model has been published in a peer-reviewed journal, the model

has a long history of use, the model has been subjected to carefully designed validation studies, and the model is supported by governmental agencies or outside experts.

Assuming that the model is found to be credible, the next steps are model calibration and validation. The purpose of model calibration is to take the generic model and, by specifying the "correct" parameter values, turn it into a predictive tool for the system of interest. Validation tests the adequacy of the calibration exercise on an independent set of data. There are numerous statistical and graphical techniques that may be used to assess how well model performance matches observations. These include lumped measures of average model goodness-of-fit, correlation measures, parametric and nonparametric statistical tests, spatial analysis of goodness-of-fit, and Bayesian measures of estimation error. Discussion of these and other quantitative methods for testing model validity can be found in Reckhow *et al.* (1990) and in a special volume of *Advances in Water Resources* (Vol. 15, 1992), which is dedicated to the discussion of validation of computer models.

Once a calibrated and validated model has been selected, the next step is to select and parameterize each of the input distributions.

7.5.4 Choosing Input Distributions

The choice of an input distribution generally depends on (i) the form of the observed data, which may be determined by graphical or statistical regression techniques, and (ii) a basic understanding of the system, which allows assessors to theorize about the distributions that will best describe the underlying reality (Table 7.2 and Figure 7.2). For example, a lognormal distribution is usually appropriate for any variable that is the product of a large number of random variables, such as concentration in a particular medium (Hattis and Burmaster 1994).

The following is a list of approaches for choosing input distributions, going from the highest degree of confidence to the lowest (adapted from Seiler and Alvarez 1996 and Moore 1996):

- *If the distribution is known for the input variable, choose it.* Typically, these variables are defined by the nature of the physical processes that lead to variability in interactions or measurements (Seiler and Alvarez 1996). An example is the binomial distribution for experiments that determine probabilities by counting certain events. Normal and lognormal distributions may be inferred from the structure of the variations in the stochastic variable. For example, if the variability arises from a sum of contributions with many variations, each with a mean and variance, the distribution of the sum is asymptotically normal. If, instead, the variability arises from the product of contributions with many variations, each with a mean and variance, the distribution is asymptotically lognormal (Ott 1995; Seiler and Alvarez 1996). Ott (1995) and the chapter by Mitchell Sharp in Morgan and Henrion (1989) discuss the theory underlying several key distributions in much more detail.

- *Use empirical data to fit a distribution.* Measurements of substances in the environment often have histograms and logit plots compatible with a lognormal distribution. Other variables may have histograms and probit plots compatible with a normal distribution. Any fitting of data to a distribution should be examined visually (e.g., probit or logit plots should produce straight lines for variables with underlying normal and lognormal distributions, respectively) and tested (e.g., the W test may be used to test whether the data were drawn from an underlying normal distribution; conducting the test on logarithms of the data will test whether the data are from an underlying lognormal distribution) (Gilbert 1987).

- *Use surrogate data to fit a distribution.* An example is the use of measured body weights of a particular mammal in a location different from the location of interest in the risk analysis. In this case, an assessor would have to justify that the extrapolation from one location to another is reasonable.

- *Use existing data to fit portions of the variable.* This situation is common in environmental assessment. The tendency when information is lacking is to use uniform and triangular distributions. Seiler and Alvarez (1996) are quite critical of the use of such distributions when information is lacking. The reason is that use of the uniform distribution, for example, implies that we know a minimum and a maximum with absolute certainty (which is rarely the case) and that all values in between are equiprobable (which is almost never the case). Often in these situations, the assessor can make better use of the available information to choose a more appropriate distribution.

Table 7.2 Useful input distributions for probabilistic risk assessments of priority substances.

Distribution	Example Applications
Beta	Modelling environmental concentrations. Rough model in absence of data.
Binomial	Number of malformations at a contaminated site.
Chi-square	Sum of weights of objects, each following a normal distribution.
Exponential	Time between events. Lifetime of organism with constant probability of mortality.
Gamma	Time to complete task. Modelling environmental concentrations.
Geometric	Number of trials until success is achieved.
Lognormal	Product of a large number of other quantities. Modelling environmental concentrations. Modelling toxicity test results with quantal data. Distribution of physical quantities in nature.
Normal	Size of quantities that are the sum of other quantities. Distribution of population characteristics.
Poisson	Number of events in a given unit of time (e.g., accidental releases).
Triangular	Distribution when minimum, maximum, and most likely values are known.
Uniform	Distribution when minimum and maximum are known and all values between are equiprobable.
Weibull	Modelling environmental concentrations. Modelling toxicity test results with continuous data. Lifetime of a device.

Choice of distribution becomes inherently more subjective as one moves down the list. Thus, the approaches at the top of the list are recommended over those at the bottom. When there is doubt about the effect of different input distributions, try each plausible distribution and note the effect on the estimates of risk. Bukowski *et al.* (1995) found that the selection of a distribution for a given input variable can have a profound effect on the risk estimate, whereas the inclusion of correlations between input variables is important only if the correlations are high and the variances large (also see Smith *et al.* 1992).

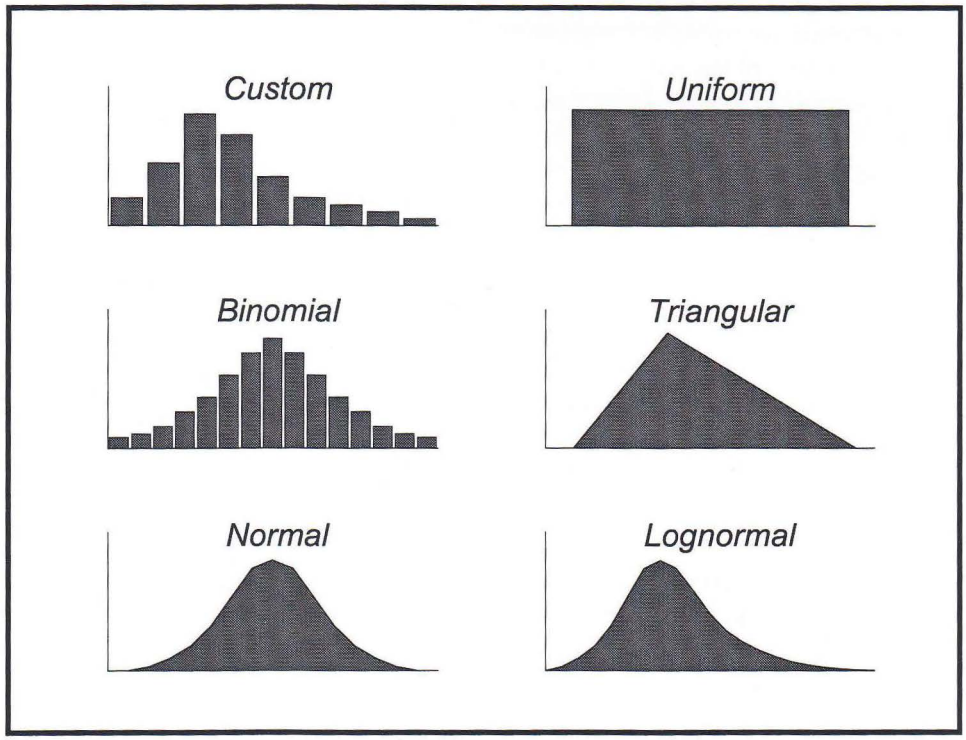

Figure 7.2 Commonly used input distributions in ecological risk assessments.

7.5.5 Methods for Probabilistic Risk Analysis

In many probabilistic risk analyses, risk curves or estimates can be derived simply by integrating an exposure and an effects distribution. Examples include scenarios where there is one dominant route of exposure (e.g., concentration in water) and a single response variable (e.g., *Daphnia* mortality; percentage of genera affected). In other analyses, risk estimates are based on more complex models (e.g., exposure from multiple media, risk cascades through a food web). This section describes probabilistic methods that may be used for both of these situations.

Estimating Risks: Analytical Methods

Analytical methods may be used to estimate risks with relatively simple model equations. The analytical method most commonly used is variance propagation (Morgan and Henrion 1989; Hammonds *et al.* 1994). If one has a simple additive model and the input variables are independent, the mean value of the output distribution is the sum of the input means. Similarly, the variance of the output distribution is the sum of the variances of the input variables. That is:

$$\mu_R = \sum_{i=1}^{p} \mu_i$$

$$\sigma_R^2 = \sum_{i=1}^{p} \sigma_i^2$$

where p is the number of variables in the model. The shape of the resulting output distribution will tend to be normal even if the distributions assigned to the inputs are not normal.

A similar approach can be taken with a multiplicative model after first converting the model to its additive form by logarithmically transforming the input variables.

$$Y = a \times b \times c$$

$$\ln(Y) = \ln(a) + \ln(b) + \ln(c)$$

For multiplicative models, the geometric mean is the exponential of the sum of the mean values of the logarithms of each input variable. The geometric standard deviation is found by taking the square root of the sum of variances of the transformed variables and exponentiating. That is:

$$X_{g,R} = e^{\mu,R}$$

$$S_{g,R} = e^{\sqrt{\sigma_R^2}}$$

where

$X_{g,R}$	=	the geometric mean of the resulting output distribution
m,R	=	the sum of the means of the logarithms of the input variables
$S_{g,R}$	=	the geometric standard deviation of the resulting output distribution
s_R^2	=	the variance of the logarithms.

The distribution of the output distribution for a multiplicative model will tend to be lognormal even when the input distributions have different shapes. Hammonds *et al.* (1994) describe variance propagation in more detail.

Estimating Risks: The WERF Approach

An approach has been developed for estimating community-level risks based on the percentage of genera affected by acute or chronic substance exposures (Parkhurst *et al.* 1996). The approach requires two types of information. The first is a distribution relating substance concentration or dose to the percentage of species or genera affected (see Figure 7.3 and Section 6.3.6 of the resource document). The second is a distribution of chemical concentrations or other measure of exposure. The two distributions are then integrated to produce a joint probabilistic risk function. The result of this analysis is a risk curve showing the probabilities of effects of varying magnitudes (i.e., percentage of genera affected). Such curves are an excellent quantitative means of describing and communicating risks. Note that the same approach may be used to estimate risks to single populations. The only difference is that the effects distribution is a concentration-response curve for the species of interest. The above equations can also be expanded to estimate risks of multiple substances that have similar modes of action. The software for the WERF approach is available upon request to the original authors.

Estimating Risks: Monte Carlo Simulation

One very commonly used probabilistic risk assessment technique in ecological risk assessment is Monte Carlo simulation. The basis for a Monte

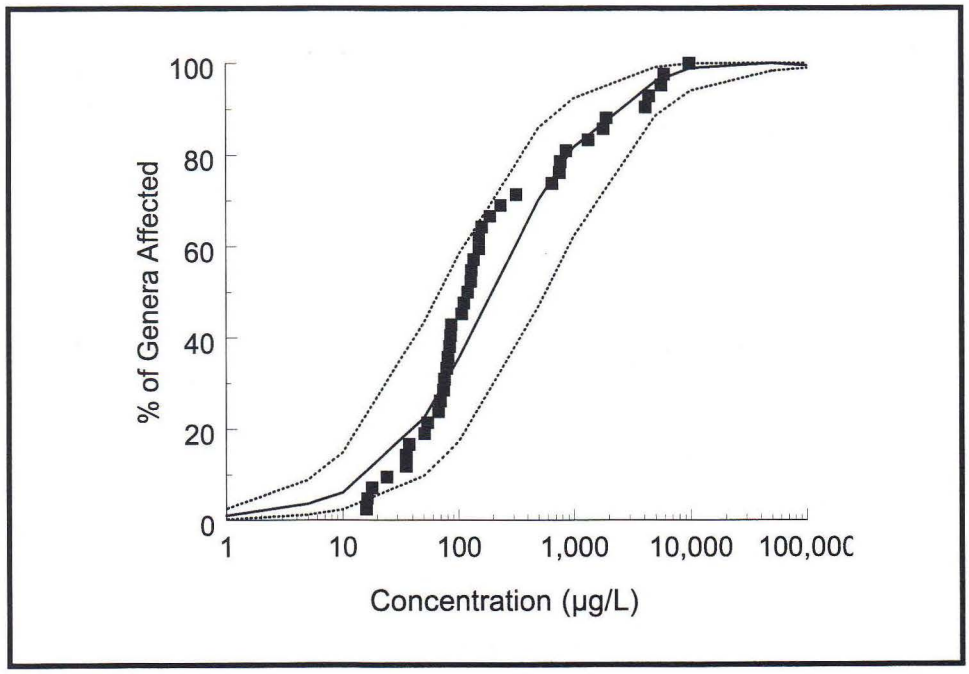

Figure 7.3 Percentage of genera affected versus copper concentration. Each point is an acute LC_{50}. A log logistic model has been fitted to the data (solid line), and 95% confidence limits have been calculated (dashed lines).

Carlo analysis is straightforward. Point estimates in a model equation are replaced with probability distributions, samples are randomly taken from each distribution, and the results are tallied, usually in the form of a PDF or cumulative density function (CDF). Several variations of the Monte Carlo technique for sampling from input distributions are available. One variation is importance sampling, in which values of particular importance (usually the tails of the input distributions) are sampled more often and then given reduced weight in order to improve resolution in the tails of the output distribution. In stratified sampling, the input distributions are divided into intervals and input values obtained by random sampling from within each interval. The most popular version of stratified sampling is latin hypercube sampling, which divides input distributions into equiprobable intervals. Latin hypercube sampling is more precise than conventional Monte Carlo sampling because the entire range of the input distributions is sampled in a more even, consistent manner (Iman and Helton 1988).

Monte Carlo techniques excel when large quantities of data and theory exist to properly specify the model equation and the input distributions. Difficulties arise when there is insufficient information to specify input distributions or the relationships between them. Dependencies between input distributions can exaggerate or reduce the predicted probabilities of effects compared with the uncorrelated case (Smith *et al.* 1992; Ferson and Long 1994; Bukowski *et al.* 1995). In cases where the dependency relationships are linear and the data exist to specify the correlation coefficients, @Risk, Crystal Ball, and other software packages have the capability to induce the dependencies in the analyses. If important dependencies are suspected but insufficient data exist to specify the relationships, then the analysis becomes problematic. In such cases, other techniques such as probability bounds analysis or fuzzy arithmetic should be considered, because the results of such analyses do not depend on knowledge about the covariance among input variables (Ferson and Kuhn 1994; Ferson and Long 1994).

Estimating Risks: Other Methods

In many cases, the paucity of empirical data will make it difficult to properly specify the input distributions. In such cases, it is inappropriate to use Monte Carlo analysis. An alternative technique is probability bounds analysis, which represents each uncertain input distribution within an entire class of probability distributions that conform with the available empirical information about the variable (Ferson *et al.* 1997). When large quantities of empirical data are available, this class may be very small. Other times, the class is very large, reflecting the poor state of knowledge about the input variable. Ferson *et al.* (1997) describe how to derive optimal bounds on the cumulative distribution functions in these classes for situations in which empirical information is limited. Once the bounds on each input distribution have been determined, it is possible to compute the bounds for the output risk curve using RiskCalc. Figure 7.4 shows the results of a risk analysis for female mink exposed to hexachlorobenzene in the St. Clair River area near Sarnia, Ontario. Input distributions for this analysis included concentrations in air, water, and selected prey items, as well as their corresponding inhalation, drinking, and ingestion rates. The figure includes the results for two estimation techniques: Monte Carlo analysis using conventional or default distributions, and probability bounds analysis. According to the Monte Carlo analysis, there is a 19% probability ([1 - 0.81] x 100) of total daily intake exceeding the 20% effect level for decline in reproductive fecundity of mink. When uncertainty concerning input distribution shapes is taken into account, however, the probability bounds analysis indicates that the probability of total daily intake exceeding the 20% effect level could range from 0 to 66%.

Other numerical methods for probabilistic risk analysis include (i) two-dimensional Monte Carlo analysis (Hoffman and Hammonds 1994) and (ii) various Bayesian methods, including Bayesian Monte Carlo (Warren-Hicks and Butcher 1996). Nonprobabilistic techniques for propagating uncertainty include interval analysis and fuzzy arithmetic (Ferson and Kuhn 1994). The choice of which method to use depends on the complexity of the risk analysis, the available information, and the expertise of the assessor. The following are

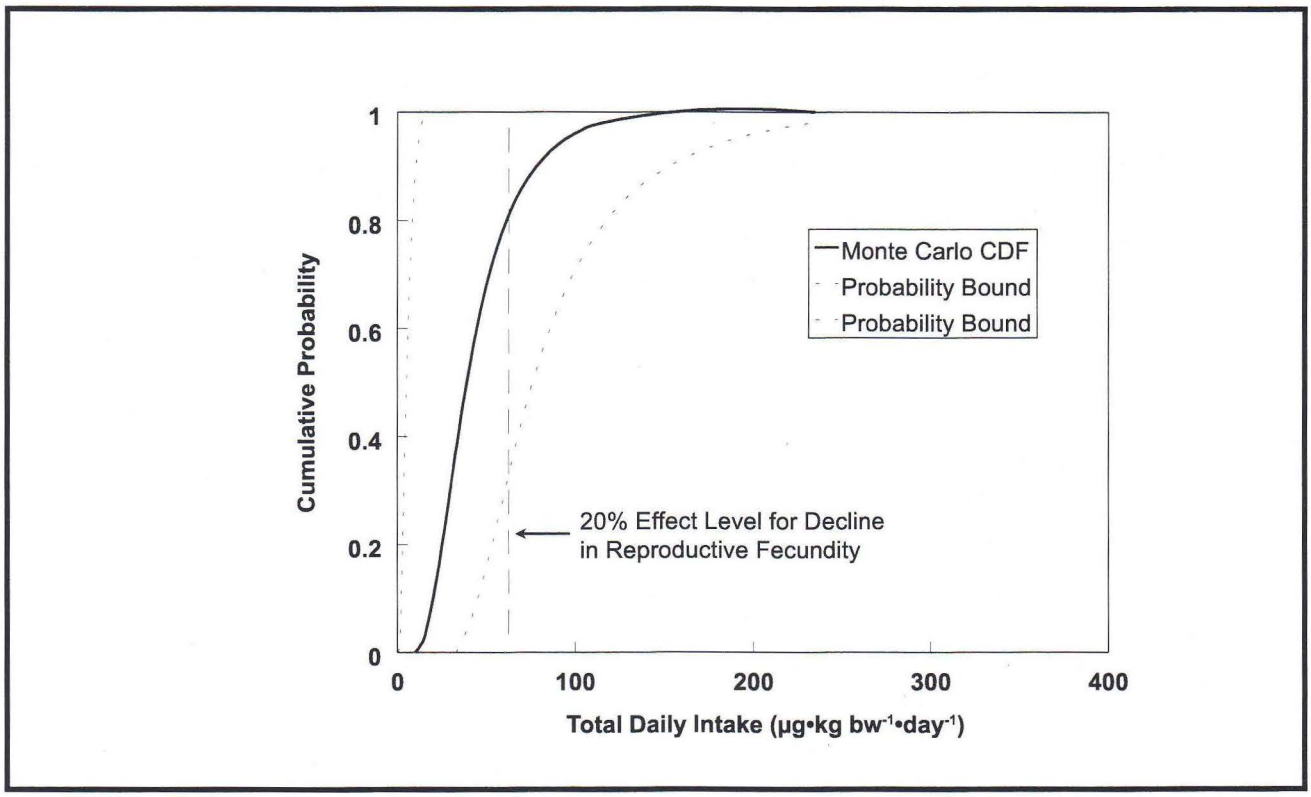

Figure 7.4 Total daily intake for female mink exposed to hexachlorobenzene in the St. Clair River area near Sarnia, Ontario. Exposure was estimated by two techniques: Monte Carlo analysis and probability bounds analysis.

general points of guidance to assist assessors in choosing an appropriate probabilistic risk analysis method:

- For simple additive and logarithmically transformed multiplicative models where the variables are independent, an analytical approach such as variance propagation is recommended.
- For more complex models, Monte Carlo simulation methods are recommended, but only if there is sufficient information to adequately characterize the input distributions and the relationships between them.
- For complex models with limited information, other methods with less restrictive requirements are recommended (e.g., probability bounds analysis, fuzzy arithmetic).

The choice of a probabilistic risk analysis method and subsequent analyses should be peer reviewed by experts.

7.5.6 Best Practices

The following 14 principles were developed by Burmaster and Anderson (1994) for Monte Carlo analysis. They have been slightly adapted here to make them applicable to probabilistic risk analyses in general. If adhered to, these principles will make probabilistic risk analyses easier to understand, will explicitly distinguish assumptions from data, and will consider and quantify effects that could lead to misinterpretation of the results. As such, it is strongly recommended that assessors follow these principles when carrying out a Tier 3 probabilistic risk analysis.

(1) Show all model equation formulae.

(2) Use point estimates as inputs before proceeding to the probabilistic risk analysis.

(3) From the results of the deterministic analysis, identify the input variables (i) that account for a dominant fraction of the predicted risks (e.g., ingestion of contami-

nated fish may be the dominant route of exposure for mink exposed to persistent organochlorines) and/or (ii) the ranges of which account for the dominant fraction of the range of predicted risks. These input variables are the ones suitable for probabilistic treatment.

(4) Restrict the use of probabilistic techniques to the pathways or sources that can potentially influence the assessment of CEPA toxicity or subsequent risk management decisions, in order to save scarce resources. For example, if conservative, deterministic calculations indicate that a quotient for a particular metal in a complex mixture is <0.01, then do not include this substance in a probabilistic analysis designed to estimate total risks from the mixture.

(5) Provide a graph showing the distribution and a table showing the mean, variance estimate, and range for each input distribution.

(6) Show how each input distribution represents variability and uncertainty.

(7) Use measured data, whenever possible, to select and parameterize inputs.

(8) Discuss the methods and report goodness-of-fit statistics for any fitted input distribution. For distributions chosen on theoretical grounds, include a rationale justifying the chosen distribution.

(9) Discuss the presence or absence of moderate ($r > 0.6$) to strong correlations, particularly if the assessment of CEPA toxicity will be influenced by the tails of the output distribution. Where such correlations exist, invoke the dependencies in the analysis using high and low estimates of the correlation coefficients to learn if the correlations influence the analysis.

(10) Provide detailed graphs and summary statistics (e.g., mean, quartiles, range) for each output variable.

(11) Perform probabilistic sensitivity analyses on key inputs in such a way as to distinguish the effects of variability from the effects of uncertainty (e.g., change uncertain inputs and rerun analyses to determine influence of lack of knowledge on the outputs). Report the results of these computational experiments.

(12) Investigate the numerical stability of the central moments and tails of the output distribution. Typically, the tails of the output distribution are less stable and more sensitive to changes in the tails of the input distributions. Because the tails of the output distribution stabilize slowly, include enough iterations to ensure stability ($\geq$10 000), or use latin hypercube sampling to stabilize the tails as quickly as possible.

(13) Present the name and statistical quality of the random number generator. Some well-known generators have short recurrence times and are thus unsuitable for Monte Carlo analysis.

(14) Discuss the limitations of the methods and of the interpretation of the results. Discuss the possible consequences of sources of uncertainty not included in the analysis, and indicate where additional research will improve the analysis.

7.6 Estimating Risks Due to Anthropogenic Sources of Naturally Occurring Substances

Risk assessments of naturally occurring substances must take into account naturally enriched areas and the tolerance of organisms occupying these areas to elevated concentrations. Such an analysis is required only when a Tier 1 risk analysis indicates a potential for harmful effects and there is evidence of areas being naturally enriched in Canada. The problem facing assessors is to evaluate the potential impacts of further increasing exposure in these areas through anthropogenic

inputs. In such cases, natural background concentrations should be estimated as precisely as possible.

If the natural background concentration of bioavailable forms of the substance exceeds the Tier 1 ENEV for sensitive endpoints, the ENEV should be refined for Tiers 2 and 3. This involves:

- defining a lower bound for the ENEV,
- evaluating the choice of assessment and measurement endpoints, and
- evaluating the relative tolerance of assessment and measurement endpoints.

These steps arose from a workshop on effects on organisms in naturally metal-enriched areas, held at Trent University in August 1995 (Hutchinson 1996).

7.6.1 Bounding the Estimated No-Effects Value (ENEV)

In areas of elevated natural concentrations of a substance, resident organisms have acquired a tolerance for the substance, whereas organisms that are sensitive to the substance are excluded from the areas. In these areas, the ENEV should not be set below the estimated natural background concentration. Unfortunately, estimating natural background concentrations in contaminated areas can be difficult. When a natural background concentration can be estimated only as a single mean value, that value may be used as the lower boundary of the ENEV. In cases where the natural background can be characterized as a distribution, the lower boundary of the ENEV should be the 90th percentile of the distribution for the area of concern.[1]

7.6.2 Evaluating the Choice of Endpoints

Organisms residing in areas where a substance is naturally enriched will have some tolerance of the substance, but the degree of tolerance may vary. Assessment endpoints should pertain to classes of organisms that are the least likely to develop high tolerance but are still relevant to the site of exposure. Potential for tolerance in different strains of a species or in related types of species may be evaluated by reviewing the literature to determine whether high effects thresholds have been reported, particularly when test organisms were preexposed to a substance. When assessment endpoints are found to pertain to a class of organisms that may be highly tolerant, different endpoints may be chosen. For example, abundance of aquatic invertebrates might be substituted for algae, if review of the literature indicates that invertebrates are much less likely than algae to develop high tolerance.

7.6.3 Evaluating the Relative Tolerance of Assessment and Measurement Endpoints

Measurement endpoints should exhibit tolerances that are similar to those of the corresponding assessment endpoints. When measurement endpoints are likely to be less tolerant than the assessment endpoints, consideration should be given to reducing or even eliminating the application factors employed to derive the ENEV. If this approach is inappropriate because of large uncertainties, new toxicity studies may be required. Ideally, area-specific organisms would be chosen for testing. A bioassay protocol for obtaining toxicity data relevant to plants inhabiting naturally enriched areas has been proposed by Hutchinson (1996).

7.7 Estimating Ecological Consequences

Estimating the probabilities of exceeding an effects threshold or effects of differing magnitudes only fulfils part of the information required for risk management decisions. This is because statistically obvious effects (e.g., high probability of a 20% decline in reproductive fecundity) may or may not be ecologically important. At the community level, a stressor-induced change in microbial species composition is not ecologically significant if there is redundancy in the functions performed by the species (Harwell *et al.* 1994).

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[1] Depending upon the shape of the natural background distribution, setting the minimum ENEV at the maximum value could result in an ENEV that is much higher than typical exposure values. Thus, using the maximum value would seem inappropriate. Alternatively, setting the minimum ENEV equal to the median natural background value would imply that assessment endpoints are adversely impacted by natural levels of the substance in up to half of the area of concern — an unlikely occurrence.

Conversely, effects on a few sensitive species might be viewed as ecologically insignificant at first glance; however, if those species are key predators or form the basis of the food chain, then the risks may cascade and lead to serious community-level impacts. Thus, risk managers and other interested parties need to know the consequences of continued exposure to the priority substance in order to better understand the substance's potential effects in the environment. Population- and community-level models and field studies may be used to explore the consequences of exposure to a priority substance. The following section describes some of the available population- and community-level field methods and models that may be used to estimate ecological consequences.

7.7.1 Population- and Community-Level Effects

Assessments of potential risks posed to populations will focus on the probability of different degrees of population reduction. Methods used to characterize such reductions may include quantitative comparison of the distribution and abundance of populations in contaminated areas with those in control or reference areas. In the absence of field data, population models may be used to predict ecological consequences.

Individual-oriented models (DeAngelis *et al.* 1991) have been developed to assess ecological risks posed to smaller populations of threatened or endangered species (e.g., Atlantic salmon; Power and Power 1994). These models permit the integration of animal behaviour, life history, biology, and ecology with degrees of realism and detail that cannot easily be achieved using more conventional aggregated models (e.g., demographics or bioenergetics models) (Power and Power 1994). The trade-off for more realism is the additional demand for model parameters. A particularly powerful and promising approach for assessing ecological risks in terrestrial systems lies in the integration of individual-oriented models with spatially explicit representations of necessary ecological resources, as well as stressors, using geographic information system (GIS) technology as an operational framework. Population models can take the form of age- or size-structured demographic models (Caswell 1989, 1996; Ferson *et al.* 1989). These models can be used to assess risks of decreased survival or decreased fecundity in relation to ecological stressors (Ferson *et al.* 1996). Demographics models have been developed to characterize the dynamics of plants, invertebrates, and mammals (see references in Caswell 1996 and Sibly 1996). Demographics models can be used to address longer-term projections of risk on future population sizes of the species of interest. Risks may be characterized as the probability of different magnitudes of population decline in comparison to baseline projections for nonstressed reference populations. There are many programs currently available that use demographics models to estimate risks to populations, including GAPPS (Harris *et al.* 1986), RAMAS/age (Ferson and AkHakaya 1990), RAMAS/stage (Ferson 1994), RAMAS/space (AkHakaya and Ferson 1992), and ALEX (Possingham *et al.* 1992). Each of these programs contains a large number of assumptions and simplistically models the behaviour of organisms. Thus, caution should be used in interpreting the results of any such analysis. In addition, no one model is best suited for all population modelling because of the diversity of life histories and population dynamics among species.

Population dynamics and risks can also be described using bioenergetics models (e.g., Bartell *et al.* 1986). Bioenergetics models can address both direct and indirect ecological effects of stressors on the accumulation and allocation of energy inputs (i.e., photosynthesis, consumption) by individual organisms from the populations of interest. Bioenergetics models are more appropriately scaled to characterize risks associated with chronic stress. These models also characterize risk as the probability of observing the effects of interest in relation to the magnitude of stress — for example, substance exposure concentrations (e.g., Bartell *et al.* 1992).

Community and ecosystem models can be used to explore how substances could affect higher-order endpoints such as community composition, productivity, and nutrient cycling. Suter and Bartell (1993) concluded that there are 15–20 aquatic and 5–10 terrestrial community and ecosystem models that could be used or slightly modified to estimate higher-order effects.

Examples include SWACOM (Bartell *et al.* 1992) and AQUATOX (Park 1996) for estimating the effects of stressors on aquatic ecosystems. Few of these models are easy to use, and few have received adequate field testing to validate model structure and predictions.

Notwithstanding the difficulties in using and evaluating models, population and community models can strengthen the weight-of-evidence determination for conclusions established by other means. They can also identify key functional and structural aspects of the system under consideration (Oreskes *et al.* 1994). For priority substances already determined to be "toxic" under CEPA, and where adequate data exist, risk assessors and managers may use appropriate population- and higher-level models to better understand the potential ecological consequences of exposure and to make effective risk management decisions. Because of the level of expertise required, assessors should work with recognized experts to carry out such analyses.

7.8 Some Points to Remember

- Present a summary statement for each of the major components of the risk assessment, along with estimates of risk, to give a combined and integrated view of the evidence.
- Clearly identify the key assumptions, their rationale, the extent of scientific consensus and uncertainties, and the effect of reasonable alternative assumptions on conclusions and estimates. In quantitative assessments, also include the rationale for model selection and information about parameter sensitivities, stochasticity, and model uncertainty (Smith and Shugart 1994).
- Outline ongoing or potential research projects that would significantly reduce uncertainty in the risk estimation.
- Provide a sense of perspective about the risk. In doing so, avoid unrelated or inappropriate risk comparisons, such as risk of mortality due to benzene exposure versus risk of mortality due to natural causes (Freudenberg and Rursch 1994; Shrader-Frechette 1995). Instead, discuss effects in terms of ecological consequences for the assessment endpoint of interest. Environmental quality guidelines or other environmental benchmarks may be useful here to help focus risk management efforts. At this point, risk assessors may wish to indicate logical groupings of substances and possible priority actions for best managing environmental risks.

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CHAPTER 8

COMPLEX SUBSTANCES

8.1 Background and General Approaches

Most of the work in environmental toxicology and environmental assessment has focused on individual substances. In nature, however, biota are often exposed to complex substances, such as mixtures or effluents.[1]

There are four types of complex substances (adapted from U.S. EPA 1986, 1988; Vouk *et al.* 1987):

- *Type 1:* those composed of related substances having similar physical and chemical properties (e.g., polycyclic aromatic hydrocarbons, or PAHs, PCBs, dioxins),
- *Type 2:* those that are generated or released at a given time and place (e.g., emissions from smelters, effluents), that have a relatively defined and constant composition, but that are not necessarily composed of related substances,
- *Type 3:* those that are commercially or chemically unrelated (i.e., having different physical and chemical properties) and that occur by coincidence at a given time and place (e.g., landfill leachate), and
- Type 4: those commercially manufactured or formulated products that serve a specific function (e.g., oil recovery mixtures, de-icing fluids, flame retardants, road salts), that have a defined and constant composition, and that are composed of unrelated substances (e.g., co-solvent carriers, surfactants, stabilizers, anti-freezes, dyes), often enhancing or imparting special properties to one or several active ingredients.[2]

The objective of this chapter is to provide guidance on how to conduct an environmental assessment of a complex substance. The chapter will focus on the differences between assessments of complex and individual substances, with particular emphasis on effects and risk characterization. Much of the guidance for assessments of individual substances addressed in other chapters of this manual also applies to assessments of complex substances. Some of this guidance is repeated in this chapter in order to present a complete overview of the assessment of complex substances. Assessors should refer to appropriate chapters when clarification or additional information is needed on a particular issue. Chapter 8 of the resource document provides additional information on the approaches and methods discussed in this chapter and guidance on the collection of data unique to complex substances.

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1 See definition in Glossary (Appendix I).

2 Active ingredients have commercially desirable attributes and are not necessarily the harmful components in the formulation, as is the case for pesticide formulations.

This chapter presents a number of approaches and methods that can be used in environmental assessments of priority complex substances. Methods for conducting the assessment are outlined in order of preference but should not be interpreted as prescriptive. Studies required to conduct environmental assessments of complex substances are not always available. In such cases, research may be required to generate the appropriate data. Research needs can be identified using appropriate models. Models that have been calibrated and validated for Canadian conditions can also be used to estimate risks. When models are used, experts should be consulted with regard to their advantages, limitations, and assumptions. Costs of generating data for preferred methods are often onerous, and data should be generated only when uncertainties around an assessment are unacceptable. Such decisions will be made on a case-by-case basis with the involvement of assessors, risk managers, and other interested parties. Regular communication between assessors and risk managers is key to decision-making regarding data generation.

For relatively simple, well-characterized effluents and mixtures for which joint toxicity or independent toxic action (see Section 8.6 in the resource document) can be assumed, an approach similar to that for individual substances may be used. For more complex substances, the tiered approach used for assessments of individual substances may be modified as required. For example, in place of using EEVs and ENEVs, results of whole-effluent or whole-mixture toxicity tests with sensitive organisms may be used for Tier 1 screening. Similarly, in some cases, results of laboratory-ambient toxicity tests (see Section 8.5.4) using samples of environmental media collected close to sources could be used for Tier 2. For example, a comparison of the toxicity test results using an ambient water sample taken upstream (i.e., control) of an effluent discharge and 50 m downstream of the discharge can provide an estimate of risk. Whenever possible, Tier 3 should take into account the spatial and temporal scales of effects, and, whenever possible, uncertainties should be quantified. A weight-of-evidence approach is recommended for complex substances (see Section 8.5.1).

A tiered approach may not be appropriate for the assessment of complex substances in all cases. For example, when data for a Tier 3 assessment are available, the assessment could proceed directly to that tier. If there is a strong suspicion that a substance causes environmental harm and research is needed to conduct the assessment, then assessors should proceed directly to higher tiers in order to determine the extent of the damage.

8.2 Problem Formulation

In problem formulation, the goals, breadth, and focus of the assessment are established, data gaps are identified, and a strategy for proceeding with the assessment is devised. This phase includes *initial scoping*, *pathways analysis*, consideration of *receptor sensitivity*, an analysis of the *ecological relevance* of potential receptors, selection of *assessment endpoints* and associated *measurement endpoints*, and the development of a *conceptual model*.

A complex substance must be thoroughly characterized in the problem formulation stage. The characterization is carried out in initial scoping and pathways analysis, where entry and exposure are identified. Ongoing refinement of this characterization may be necessary throughout the assessment process as additional data are obtained.

During initial scoping, the characterization involves identifying various technical names of the substance and, on a qualitative basis, identifying major constituents, potential constituents of concern (such as substances previously determined to be CEPA "toxic"), group parameters,[3] and predetermined sources of release.

[3] Group parameters are based on analytical-chemical techniques and determine specific elements or chemically defined groups of constituents in complex substances. Examples of group parameters are dissolved organic carbon (DOC) and Adsorbable Organic Halogen (AOX).

In pathways analysis, data needed to characterize environmental releases for complex substances include volumes, flow rates or quantities released, location of releases, receiving environment characteristics, temporal patterns of release, and other information on the life cycle of the complex substance released to the environment.

Once the substance and its release are sufficiently characterized, its environmental partitioning, fate, and geographic distribution should be determined. To do this, data are needed on chemical monitoring of constituents and group parameters obtained from field and laboratory studies involving chemical analysis (see Sections 8.4 and 8.5). Physical and chemical properties of constituents and group parameters indicate possible fate, transport, and composition of the complex substance following release. Models can also predict the environmental fate of complex substances. The behaviour of complex substances cannot necessarily be predicted based on the behaviour of the individual constituents. Data on physical and chemical properties, interactions between constituents, and interactions between constituents and the receiving environment are often unavailable. Such modelling approaches may, therefore, be used only for a qualitative fate assessment.

Understanding how constituents and group parameters in complex substances behave is essential in considering receptor sensitivity, identifying assessment and measurement endpoints, and assembling a conceptual model. Examples of measurement endpoints that have been used in bioassays of complex substances (types 1–4) are presented in Table 8.1 of the resource document.

Organisms selected as the ecological component of assessment endpoints should be among those most at risk because of high exposure to the complex substance. Potential for exposure should be based, if possible, on the following factors: (i) knowledge about how the constituents are distributed in the environment, (ii) major routes of exposure for different types of organisms, and (iii) the spatial and temporal distributions of potentially exposed organisms in Canada. In doing so, this will ensure that the organisms selected are likely to have been present in the areas of concern prior to the onset of contamination. Other factors that affect exposure, such as diet, mobility, and body size, should also be considered when selecting assessment endpoint organisms.

8.3 Entry Characterization

Entry characterization identifies sources of release and quantifies the amounts released to the Canadian environment using a life cycle approach.

Sources can be identified by updating a substance's life cycle and by identifying domestic and transboundary sources of entry. A life cycle approach may not be necessary for substances with predetermined sources of release (e.g., air emission from a specific smelter). Once the sources of release have been identified, entry characterization should focus on a quantitative analysis of the release characteristics and on refining pathways analysis.

8.4 Exposure Characterization

Exposure characterization quantifies the relationship between source inputs of a complex substance and its resulting geographic distribution in space and time (spatial and temporal scale) and identifies and quantifies exposure for populations at risk.

For complex substances, measures of exposure include constituents and/or group parameters that determine the fate and spatial and temporal scales of the assessment. Such data are also used in the effects and risk characterizations.

Monitoring of major constituents and/or group parameters is the preferred approach to quantitatively determine the fate of the complex substance and the spatial and temporal scales of the assessment. Monitoring variables should include constituents and/or group parameters that are potential causal agents of environmental effects. When monitoring studies are unavailable, data may be obtained from field and laboratory-ambient toxicity tests involving chemical analysis. In the latter type of study, samples of media are taken from the receiving environment at various distances from the point of release for chemical analysis and toxicity bioassays. Results from field and laboratory-ambient toxicity tests can help

determine the potential for exposure at a given distance from the release point and can be used directly in the effects and risk characterizations.

Models can be used to predict the environmental fate of complex substances. The usefulness of their outputs is based on the same considerations noted previously.

Exposure characterization should also focus on refining/confirming the selection of assessment endpoints. Factors to consider when assessing potential for exposure are presented in Section 8.2.

8.5 Effects and Risk Characterizations

Risk characterization determines whether complex substances are causing adverse effects on exposed organisms. By chemically characterizing a complex substance in field toxicity testing, artificial system testing, and laboratory-ambient toxicity tests, exposure and effects data can be used directly to conduct a risk characterization. Such methods minimize uncertainty of extrapolation.

The environmental assessment of complex substances can have several complications, including partitioning and persistence of constituents of complex substances after their release in the environment and additive versus interactive effects among constituents, such as antagonistic or synergistic effects. The effects of one constituent may influence the kinetics of uptake, metabolism, and excretion of other constituents. Because of these factors, complex substances may require different methods for assessing ecological risks.

The preferred methods for this phase of the assessment are presented below. These methods are listed in decreasing order of preference. It is emphasized that the order is preferred for assessing complex substances and should not be interpreted as the order in which data may need to be generated when these are lacking:

(1) field toxicity tests (e.g., *in situ* biological testing, community surveys),

(2) artificial system tests: microcosm and mesocosm tests using spiking with complex substances,

(3) laboratory-ambient toxicity tests, and

(4) laboratory toxicity tests using whole-effluent or whole-mixture samples.

Constituents of complex substances often partition into different environmental compartments, such as soil, water, sediment, biota, and air, and single-species tests are customarily conducted in only one of these compartments. Field studies at the community and ecosystem levels generally provide a more realistic assessment of effects (Vouk *et al.* 1987). Such studies are often unavailable, however, and other types of field toxicity tests, including population-level studies and *in situ* bioassays, can be useful. The advantages of field toxicity tests, microcosm/mesocosm tests, laboratory-ambient toxicity tests, and whole-effluent and whole-mixture tests are outlined in the resource document (Section 8.6).

In order to use such methods, assessors must demonstrate that the observed effects are due to the complex substance and not to substances released from other sources. Assessors should always try to determine the constituents and group parameters responsible for environmental effects. Such data may not always be available using the above methods. Other methods that can identify and assess the potential adverse effects of constituents include:

- various effluent and mixture fractionation methods (e.g., toxicity identification and evaluation, or TIE),
- the individual substance method
  - similar joint action or toxic unit (TU) approach
  - independent joint action,
- the representative substance class method,
- the WERF approach, and
- the toxic equivalent factors (TEF) method.

These methods are briefly presented in Section 8.5.6 of this manual. Additional information on these methods is described in Section 8.6.5 of the resource document.

8.5.1 Weight-of-Evidence Approach

Although field toxicity tests, artificial system tests, laboratory-ambient toxicity tests, and whole-effluent and whole-mixture toxicity tests are useful methods to assess complex substances, assessors should, whenever possible, use a combination of these methods to increase confidence in the risk assessment conclusions. Other methods (noted above) can also be used in a weight-of-evidence approach. Integrating or combining methods to assess adverse effects of complex substances has been recommended elsewhere (U.S. EPA 1991; Adriaanse *et al.* 1995; De Zwart 1995; Groot and Villars 1995; Tonkes *et al.* 1995; van Loon and Hermens 1995).

Methods for directly determining the effects of complex substances on the structure and function of natural populations, communities, and ecosystems are available but are not as standardized as are the protocols for laboratory tests. A variety of methods and comprehensive frameworks are available to assess the impacts of complex substances on the receiving environment. Examples are the Environmental Effects Monitoring Program and the Canadian Environmental Assessment Research Council (CEARC) approach (Peterson *et al.* 1987; Sonntag *et al.* 1987; CEARC 1988). These frameworks are not entirely compatible with the assessment of priority substances under CEPA, but their underlying concepts and methodologies should be considered for complex substances. The sediment quality triad approach is an example of a structured, integrative method of determining sediment contamination and assessing complex substances in sediments (Chapman 1986, 1989).

Integrated methods can be used at the population and community levels. The methods combine habitat quality and higher organizational level indices. They can be used as part of a weight-of-evidence determination, improving on decision-making and on the current understanding of higher-order ecological systems. An example is the Integrated Biotic Index (IBI), which can be used along with Habitat Suitability Indices as an ecological tool to evaluate biological conditions in streams to which effluents are discharged (Karr 1981). The methods are described in Section 8.6 and Appendix VII of the resource document.

8.5.2 Field Toxicity Tests

The main difference in designing approaches to assess the environmental risk of mixtures compared with effluents is that effluents are usually discharged to water systems, whereas mixtures can be discharged to various environmental compartments, including air, land, and water. Therefore, the experimental design of the preferred methods will depend not only on the use, physical and chemical properties, and ultimate fate of the mixture, but also on the type of receiving environmental compartment.

Aquatic Ecosystems

Factors to consider when evaluating the results of field tests are discussed in Section 8.7.1 of the resource document.

The use of spatial and temporal controls is necessary in the experimental design. The recommended field tests used to determine if a complex substance is harmful to the environment are presented below:

- Spatial Controls
  - *in situ* toxicity studies using caged organisms located upstream (control) and downstream of the discharge.
  - upstream control locations and several downstream locations at different distances from the point source. If the measure of effects increases at the point source and declines monotonically as distance from the point source increases, then there is strong evidence that the effluent or mixture is causing an adverse effect.
  - surveys of community structure, population survival, or other biological endpoints upstream and at several sites downstream from the discharge.
- Temporal Controls
  - *in situ* toxicity studies (e.g., Before–After–Control–Impact, or BACI, design) using caged organisms located upstream and downstream of the discharge and conducted before and after a process change (e.g., switching to discharges of nonchlorinated effluents).

- surveys of community structure, population survival, or other biological endpoints conducted before and after a process change upstream and downstream of the discharge.

The difference between complex substances discharged to lentic systems (i.e., having continuous water flow systems, such as rivers) and lotic systems (i.e., having little or no water flow, such as lakes and harbours) is choosing a proper control site for lotic systems (as there are no upstream sites) for both the *in situ* toxicity tests and community and population surveys. The control sites must have characteristics — such as naturally occurring biota, physical and chemical properties of the sediments and water — similar to those of the affected study sites.

When burning WCOs, emission particulates are deposited on nearby soil and vegetation. Effects can be determined on a qualitative or quantitative basis using spatial and temporal controls. A qualitative assessment could involve observations on the colour and size of affected vegetation and comparison with those of background (control site) vegetation. A quantitative analysis could involve a biological survey (e.g., species composition) of vegetation or invertebrates living in soil and comparison of results with those of background findings; in doing so, effects can be determined when, for example, tolerant species have replaced sensitive species. Another example of the use of spatial controls is to conduct *in situ* toxicity tests using caged organisms downwind of the emission and comparing responses with those of a control site. Choosing a control site for discharges or transportation of complex substances is likely to be more difficult in terrestrial ecosystems than in aquatic systems. To do this, analysis of wind currents may be necessary. When there is no consistent wind current direction, a background or control site should have physical, chemical, and biological characteristics similar to those of the affected site. Examples of temporal controls using the same scenario include (i) comparing *in situ* toxicity results before and after a process change (BACI method, see Section 8.6.3 of the resource document) and (ii) comparing toxicity test results using current levels of constituents in the vicinity of the emission and background levels acquired before the facility was constructed (BACI method). Factors that can influence results in this scenario are variability in emission rates and in composition and wind currents.

Table 8.1 Approaches and type of controls to conduct field toxicity studies of waste crankcase oils (WCOs).

Scenario	Approach	Control
Burning as fuel	*In situ* tests using caged organisms in fields	Spatial and/or temporal controls
Disposal to land	*In situ* tests using vegetation and/or microorganisms	

Terrestrial Ecosystems

As approaches used to determine the environmental risks of mixtures are designed on a case-by-case basis, examples using waste crankcase oils (WCOs) are presented below (Environment Canada and Health Canada 1994). During the WCO assessment, an attempt was made to follow its life cycle from the point of collection to ultimate disposal. Two scenarios outline ways in which WCOs enter the Canadian environment — burning and land disposal (Table 8.1). The examples are not meant to be an exhaustive list of approaches. Rather, they help illustrate experimental design that can be used to assess the environmental risk of mixtures. Expert judgment must always be used when designing an approach to assess a particular mixture. Factors to consider when evaluating the validity of the results of field tests are discussed in Section 8.7.1 of the resource document.

In the disposal to land scenario, temporal controls can be used by conducting a biological survey of microorganisms or by monitoring functional aspects of the ecosystem before and after application of WCOs (BACI method). Spatial controls can be used for volatile constituents and constituents transported by particulate matter to nearby vegetation. In this scenario, an analysis of wind currents may also be necessary to determine an appropriate control site. Comparing species composition of the affected populations with that of the controls can determine if adverse effects have occurred. Examples of adverse effects could involve differences in growth or in reproduction between the populations of concern and the controls.

Whenever possible, uncertainties associated with each scenario should be quantified.

8.5.3 *Artificial System Tests (Mesocosms and Microcosms)*

Artificial systems may be used for functional (various rate processes) and structural (species composition, richness, etc.) measurements and simple toxicity test measurements (e.g., lethality). The systems can be used for assessing effects of effluents and mixtures. Artificial system tests can also contribute to the understanding of the effects of complex substances and constituent interactions if chemical transformation and partition kinetics are measured simultaneously with structural and functional responses of the system (Vouk *et al.* 1987).

Artificial system tests are very useful when it can be demonstrated that concentrations of harmful constituents and group parameters measured in the test systems also exist in the field. In doing so, an estimation of risk can be determined.

It is recommended that these tests be verified for experimental QA/QC and for proper design in order for these to best reflect natural ecosystems. Refer to Section 6.2 of the guidance manual and Section 6.2.2 of the resource document for additional information on mesocosm and microcosm tests.

8.5.4 *Laboratory-Ambient Toxicity Testing*

Information on methods for measuring the acute or chronic toxicity of effluents and receiving waters to freshwater or marine organisms is available (Environment Canada 1990a, 1990b; Klemm *et al.* 1991; Lewis *et al.* 1991; Weber 1991; De Zwart 1995). This information can be used when evaluating the QA/QC of a study. Factors to consider when evaluating the validity of results from laboratory-ambient tests are discussed in Section 8.7.1 of the resource document.

Laboratory-ambient toxicity testing for effluents involves taking samples of receiving water or sediments upstream (controls) and at various distances downstream of the point of discharge and conducting laboratory toxicity tests on the samples. For mixtures, adverse effects can be determined by collecting air, soil, or water samples containing constituents of the mixture from various sites near the release and conducting toxicity tests on the samples. Chemical analyses (e.g., extraction, fractionation) and laboratory toxicity tests on the elutriate fractions can further characterize the components of the complex substance that is responsible for causing environmental harm. Whenever possible, uncertainties associated with determining risk to the environment using these methods (e.g., variability in effluent or mixture composition and quantity, flow, and quality of the receiving water, leachate plumes, extrapolation from the measurement to the assessment endpoint and to chronic exposure effects) should be quantified.

Using the scenarios presented in Table 8.1, laboratory-ambient toxicity tests for complex mixtures could involve the collection of particulates near facilities burning WCOs. Using these samples, deposition levels of WCO constituents could be determined and applied to laboratory biota. In this example, deposition levels could be collected over a specified time period or per volume of WCOs burned and applied to vegetation living near the facility. Another possibility could involve the collection of contaminated sediments from nearby streams where road runoff of WCOs has accumulated. Laboratory toxicity tests using these samples and local benthic invertebrates could determine the mixture's potential adverse effects and risks and provide data on fate and exposure.

8.5.5 *Laboratory Toxicity Testing Using Whole Effluent and Mixtures*

Whole-effluent or whole-mixture toxicity tests are usually conducted in the laboratory and involve either short-term (acute) or long-term (chronic) exposures.

Toxicity can be measured by using effluent samples obtained at the point of discharge and by conducting toxicity tests on the samples. This approach can be used as a hyper conservative scenario to screen effluents for potential toxicity (i.e., effects at 100% effluent concentration). If no toxicity is observed, no adverse effects are expected to occur downstream of the discharge. When effects are observed, dilutions of the 100% effluent can be used to estimate, for example, an LC_{50}. The sources of uncertainty in this approach include the extrapolation from the measurement to the assessment endpoint and to chronic exposure effects. Whenever possible, these should be quantified. Extrapolation to chronic exposure effects may be unnecessary if the effluent constituents or group parameters have a short half-life (e.g., total residual chlorine for chlorinated wastewater effluents).

Characterizing risk involves linking the inherent toxicity of the effluent, as measured in the laboratory, to concentrations in the environment and demonstrating that the assessment endpoint organisms are exposed or have the potential to be exposed to the effluent or its constituents. To do this, it must be demonstrated that concentrations of harmful constituents and group parameters measured in the dilution samples also exist in the field.

In the case of mixtures, whole-mixture samples are used directly in laboratory toxicity testing. Examples include applying WCOs directly to the organisms likely to be exposed (e.g., bird eggs), feeding organisms diets containing WCOs, or applying WCOs to laboratory soil plots to observe the response of organisms living in the soil. This approach can be used as a worst-case scenario to determine potential adverse effects. If adverse effects are observed, assessors must demonstrate that the receptors of concern have the potential to be exposed to the whole mixture. Such data can then be used in risk characterization.

8.5.6 *Other Methods*

The following methods can be applied to both effluents and mixtures. The methods discuss analytical identification and fractionation procedures for complex substances and subsequent determination of fraction toxicities. Also discussed are methods that quantitatively characterize and communicate environmental risk at the population or community level.

Fractionation procedures for a complex substance involve a separation of constituents that have similar physical and/or chemical properties. These are referred to collectively as group parameters. Aqueous or organic solutions of organic constituents are separated into elutriates using techniques such as high-performance liquid chromatography or ultrafiltration. These elutriates contain defined groups of related constituents and can then undergo toxicological testing. Fractions determined to cause adverse effects can be either chemically analyzed to identify harmful constituents or further fractionated and tested to more precisely identify harmful constituents. This method is often referred to as TIE.

When the chemistry and toxicology of the constituents have been characterized, the individual substance method can be used to calculate the total effect of the complex substance. Consideration of the possible interactions between constituents and between their effects on the exposed organism is required. Constituent interactions in complex substances can be determined by two types of noninteracting joint actions: (i) similar joint action or concentration addition, where constituents act independently to produce similar biological effects so that the concentration of one constituent can be expressed in terms of another, and (ii) independent joint action, where constituents act on different biological systems or affect the same biological system differently owing to different modes or sites of action (Mumtaz *et al.* 1994). With similar joint action, the toxicity of a complex substance can be determined by identifying constituents with similar modes of action and by calculating their joint toxicity. To do so, the ratio of each constituent concentration (EEV) and toxicity (ENEV) is calculated. Each ratio is termed the TU and can be summed. With independent joint action, the

model assumptions are that constituents have independent modes of action and the susceptibilities of organisms to different constituents are the same. By assuming no combined effect, the toxicity is the highest TU associated with the complex substance; the highest TU alone can be used to characterize the risk associated with exposure to the complex substance.

In the representative substance class method, a complex substance can be qualitatively analyzed and a representative constituent identified as being of biological significance from each class of constituents. Toxicological testing is conducted with each representative constituent, and its effects are assumed to represent the constituent class as a whole (Parkhurst 1986).

The WERF approach estimates community-level risks based on the percentage of species (or genera) affected by acute or chronic chemical exposures from multiple substance exposure (Parkhurst *et al.* 1996). The approach assumes that two pieces of information are available. The first is a distribution relating substance concentration to the percentage of species (or genera) affected (i.e., concentration vs. percentage of species affected). The second piece of information is a distribution of substance concentrations in the appropriate environmental compartment. The two distributions are integrated algebraically to produce a joint probability function. The result of this analysis is a risk curve showing the probabilities of effects of varying magnitudes (i.e., percentage of taxa affected). Such curves are an excellent quantitative means of describing and communicating risks. Refer to Section 6.3.2 of the guidance manual and Section 6.3.6 of the resource document for additional information on the WERF approach.

Another method for interpreting interactions is the TEF method. Toxic equivalent factors make use of the dose addition and potentiation concept, where constituent concentrations in a complex substance are simply added to each other (with an appropriate potentiation factor) because they have similar modes of action (U.S. EPA 1989). The approach can be used for dioxins and furans and other complex substances, such as PAHs and PCBs.

8.6 References

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