SOUTH AFRICAN WATER QUALITY GUIDELINES FOR FRESHWATER ECOSYSTEMS – VERSION 2
Volume 1: Technical Report

ON Odume, NJ Griffin, PK Mensah, D Forsyth, L Ncube and HJ van Niekerk

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South African Water Quality Guidelines for Freshwater Ecosystems – Version 2

Volume 1: Technical Report

Report to the
Water Research Commission

by

ON Odume[1], NJ Griffin[1], PK Mensah[1,3], D Forsyth[1], L Ncube[2] and HJ van Niekerk[2]

[1]Institute for Water Research, Rhodes University
[2]Department of Environmental Sciences, University of South Africa
[3]Department of Fisheries and Aquatic Sciences, University of Cape Coast, Ghana

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Water Research Commission
Bloukrans Building, Lynnwood Bridge Office Park
4 Daventry Street
Lynnwood Manor
PRETORIA

orders@wrc.org.za or download from www.wrc.org.za

Download the DSS from here: https://www.ru.ac.za/iwr/resources/software/wqgdss/

This report forms part of a set of two reports. the other report is *South African Water Quality Guidelines for Freshwater Ecosystems – Version 2. Volume 2: Implementation Manual.* (WRC Report No. TT 936/2/23)

EXECUTIVE SUMMARY

The 1996 Water Quality Guidelines for Aquatic Ecosystems are widely used in South Africa, and even beyond the borders of the country. They have also aided the management of water quality in the country, including being used for education purposes. However, they have been criticised for four fundamental reasons. First, they have been criticised for not being explicitly risk-based and not taking an explicit risk approach in their development and implementation. An important implementation outcome of not being risk-based is what has been referred to as over- or under-protection. In this regard, current guidelines are being used as trigger value, above which an action, usually corrective one, needs to be taken, and below which all is assumed to be fine, and no action may be taken. Second, they are largely generic, and not site-specific (with the exception of a few variables such as conductivity, pH, total dissolved solids, water temperature) or do not consider the spatial variability that naturally impact water quality. Third, the 1996 guidelines were developed prior to the promulgation of the National Water Act, as a result, the guidelines do not reflect the thinking informing the various resource directed measures (RDM). For example, the current guideline for freshwater ecosystems follows the trigger value approach (target water quality range), which is not very helpful given that the Department of Water and Sanitation (DWS) approach accords water resources different levels of protection, e.g. Class I, II, III and Ecological Categories A-D, with descriptive and quantitative Resource Quality Objectives (RQOs). Fourth, since the 1996 guidelines were published, much research has been undertaken locally and internationally in the field of water quality and new and emerging pollutants of concerns. There is thus a need to update the guidelines to reflect new science in the field.

The hard-copy, paper-based 1996 guidelines were deemed as not supporting rapid decision making processes and were not easily updatable. To this end, the stakeholders in the sector recommended the development of an updatable software-based decision support system (DSS) that allows rapid decision making regarding the risk posed by pollutants of concern. A multi-tier approach was also recommended for the revision of the guidelines.

Project Aims

The following were the aims of the project:

1. Review international and national application of risk-based guideline development.
2. Develop a database of spatially referenced data for South Africa, ideally at the quaternary catchment level.
3. Identify requirements for aquatic ecosystem water quality guideline revision.
4. Develop SSD curves for representative taxa exposed stressors selected for guideline revision.
5. Produce and pilot test a software product for aquatic ecosystem water quality guidelines.
6. Finalize aquatic water quality guidelines following user input and with suitable documentation for use.
7. Make recommendations for further research.

The revised Guideline follows a **multi-tier approach**, Tiers 1-3, where Tier 1 are generic guidelines developed mainly using toxicological data, generated through an SSD curve (species sensitivity distribution). The guidelines at Tier 1 are generic, conservative and are similar to the 1996 Guidelines, but with reference to the Ecological Categories A-F. The guidelines are thus aligned with the Ecological Categories. Tier 1 guidelines are developed for 23 inorganic salts; 42 organic compounds; and 26 pharmaceuticals. Temperature guidelines defer to the work of Rivers-Moore and Dallas.

Tier 2 guidelines are derived at ecoregion level II to account for spatial variability within the country. By developing guidelines for each level II ecoregions within the country, the spatial variability driven by several factors such as climate, physiography, geology and soils as well as altitude, are thus accounted for in the revised guidelines. In addition, guidelines at Tier 2 are developed for both physico-chemistry and macroinvertebrate response, thus accounting for community-based effect of the ecosystem to water quality change. The physico-chemical variables for which guidelines have been developed at Tier 2 was driven mainly by available data within the current DWS water quality monitoring networks. As such, some ecoregion level II were data-rich, whereas others were data-poor.

Tier 3 assessment is triggered when an unacceptable risk is suspected based on the results of Tiers 1 and 2. Tier 3 provides a means for a site-specific water quality risk assessment by collecting detailed site-specific information. A key feature of Tier 3 assessments is that they are event/scenario-based. The reasoning behind this approach is that improving water quality implies a focus on the event/scenario driving water quality change.

For the purpose of Tier 3 assessment, risk is conceptualized as a measure of the likelihood (probability) of an event/scenario/issue occurring and its adverse effects or consequence as well as the associated uncertainty. The Guidelines are implemented within an updatable software-based decision support system (DSS) flexible enough to allow for rapid decision making regarding the risk posed by pollutants of concern. The DSS interface allows for easy navigation. As the Guidelines are software-based, they are easily updatable, supports educational and research purposes and can also facilitate rapid decision making. Crucially, the revised guidelines can also support water quality licensing and similar imperatives.

Recommendations
The following recommendations are made:

1. **Capacity building** – As the revised guidelines have been developed using a different approach and within a new decision support system (DSS), there is a need for capacity building across various sectors of society. Such capacity building would facilitate the use of the guidelines in different contexts and by different sector stakeholders.

2. **Invest in water quality monitoring and data:** While much efforts have gone into water quality monitoring within the country, the current study suggests that additional investment is needed in water quality data collection, including establishing additional monitoring networks and building capacity within DWS, its agencies as well as other institutions responsible for data collection at local and catchment scales.

3. **Risk-based decision making:** Risk is an important element in water resource decision making. With the developed DSS, water resource managers and practitioners can assess acceptable level of risk given protection level and other resources. It is thus important that policies within the sector should place a premium on risk-informed decision-making in ways that ensure balanced use and protection of water resources, and capacity should be strengthened in this regard.

4. **New and emerging pollutants of concerns –** Although the revised guidelines now include an extensive list of chemicals previously not included in the 1996 Guidelines, research is needed in the field of new and emerging pollutants of concerns such as plastics, and their ecological effects.

Download the DSS from here: https://www.ru.ac.za/iwr/resources/software/wqgdss/

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Reference Group	Affiliation
Bonani Madikizela	Water Research Commission (Chairperson)
Akhona Mkonde	University of South Africa
Indrani Govender	Durban University of Technology
Patsy Scherman	Scherman Environmental cc.
Janine Adams	Nelson Mandela University
Pieter Viljoen	Department of Water and Sanitation
Jackie Jay	Department of Water and Sanitation
Ntuthuko Masikane	University of Zululand
Helen Dallas	Freshwater Research Centre
Sonwabile Rasmeni	National Nuclear Regulator
Christa Thirion	Department of Water and Sanitation
Nyamande Tovhowani	Department of Water and Sanitation
Gerda Kruger	Water Research Commission

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CONTENTS

EXECUTIVE SUMMARY iii

ACKNOWLEDGEMENTS v

CONTENTS vii

LIST OF FIGURES viii

LIST OF TABLES viii

ACRONYMS & ABBREVIATIONS x

CHAPTER 1: INTRODUCTION.. 1
1.1 INTRODUCTION 1
1.2 PROJECT AIMS 3
1.3 SCOPE AND LIMITATIONS 3

CHAPTER 2: LITERATURE REVIEW.. 4
2.1 RISK CONCEPTUALISATION 4
2.2 REVIEW OF INTERNATIONAL GUIDELINES 5

CHAPTER 3: SOUTH AFRICAN WATER QUALITY GUIDELINES FOR FRESHWATER ECOSYSTEMS: VERSION 2 – TIER 1 11

3.1 INTRODUCTION 11
2.2 METHODOLOGY..11
3.2.4 Implementation 18
3.2.5 Ecological Categories 18
3.2.6 Tier 1 Guidelines..19

CHAPTER 4: SOUTH AFRICAN WATER QUALITY GUIDELINES FOR FRESHWATER ECOSYSTEM: VERSION 2 – TIER 2 20

4.1 INTRODUCTION 20
4.2 DERIVATION OF PHYSICO-CHEMICAL GUIDELINES AT TIER 2..20
4.3 MACROINVERTEBRATE RISK MODEL 23
4.3.1 Macroinvertebrate-based guidelines 26

CHAPTER 5: SOUTH AFRICAN WATER QUALITITY GUIDELINES FOR FRESHWATER ECOSYSTEM: VERSION 2 – TIER 3 27

5.1 INTRODUCTION 27
5.2 SITE-SPECIFIC WATER QUALITY RISK ASSESSMENT MODEL 28
5.2.1 Consequence sub-model..28
5.2.2 Likelihood sub-model: 30
5.2.3 Risk rating 31
5.3 UNCERTAINTY SUB-MODEL..32
5.3.1 Overall uncertainty/confidence rating 36

REFERENCES 37

LIST OF FIGURES

Figure 2.1 Risk matrix based on the likelihood and consequence dimensions of risk…………………………..4

LIST OF TABLES

Table 3-1 Compounds included in the Tier 1 guidelines. 21

Table 3-2 List of salts or compounds that were used to generate SSD curves for compounds of elements where simple direct toxicological data were limited or not available. 21

Table 3-3 Guideline derivation for application to SSD consensus model fits. Corresponding to generic ecological categories of Kleynhans and Louw (2007). NB x, is the guideline value at a given ecological category, and +y is the upper predicted confidence interval, and -y is the lower predicted confidence interval.. 24

Table 4-1 Guideline values for nutrients and common salts at ecoregion level 2, corresponding to generic ecological categories of Kleynhans and Louw (2007). 28

Table 4-2 Confidence level associated with ecoregion level 2 guideline values.. 29

Table 4-3 Guideline values for dissolved oxygen at a range of different temperatures in freshwater. 30

Table 4-4 Guideline values for pH at ecoregion level 2, corresponding to generic ecological categories of Kleynhans and Louw (2007). 30

Table 4-5 Conceptualised relationship between taxon ecoregional confidence weighting and macroinvertebrate risk weighting. 31

Table 4-6 Geomorphological zonation of South African river channels (Rowntree et al., 2000). 31

Table 4-7 Conceptualised relationship between taxon geozone confidence weighting and macroinvertebrate risk weighting. 31

Table 4-8 Conceptualised relationship between macroinvertebrate water quality sensitivity and risk/impact to the resource. 32

Table 4-9 Guideline derivation for Ecoregion level 2 and geozone macroinvertebrate risk estimates, corresponding to generic ecological categories of Kleynhans and Louw (2007). 34

Table 5 1 Physical chemical severity rating based on the Percent Time Equal or Exceeded rating 34

Table 5-2 Macroinvertebrates severity rating as a function of the extent of deviation between the expected and observed taxa returned by the macroinvertebrate risk model in Tier 2.. 29

Table 5-3 Rating for the duration aspect of the consequence sub-model... 30

Table 5-4 Rating for the spatial scale dimension of the consequence sub-model. 30

Table 5-5 Rating for frequency of occurrence of the risk-triggering event. 31

Table 5-6 Rating for frequency of impact of the risk-triggering event. 31

Table 5-7 Rating for the detection of the risk-triggering event or its impact on the water quality component of the resource. 31

Table 5-8 Overall site-specific risk rating based on the consequence and likelihood sub-models. 32

Table 5-9 Uncertainty scoring regarding the reliability and reasonability of the assumption of the risk-triggering event(s). 34

Table 5-10 Uncertainty scoring associated with the physico-chemical severity dimension of site-specific risk assessment. 34

Table 5-11 Uncertainty scoring associated with the macroinvertebrate severity dimension of site-specific risk assessment. 35

Table 5-12 Assessing the level of expert agreement/disagreement/literature support at Tier 3 site-specific risk assessment. 35

Table 5-13 Uncertainty assessment regarding the risk assessor's knowledge of the site-specific risk modifying factors. 36

Table 5-14 Overall uncertainty rating associated with the site-specific water quality risk assessment. 36

ACRONYMS & ABBREVIATIONS

ACWUA	Assessment of Consideration for Water Use Application
ANZG	Australian and New Zealand Governments
ATC	Anatomical Therapeutic Chemical Classification System
BLM	Biotic Ligand Model
CAS	Chemical Abstracts Service
CCC	Criterion Continuous Concentration
CCME	Canadian Council of Ministers of the Environment
CEQG	Canadian Environmental Quality Guidelines
CMC	Criterion Maximum Concentration
CWQGs-PAL	Canadian Water Quality Guidelines for the Protection of Aquatic Life
DSS	Decision Support System
DVG	Default Guideline Values
DWA	Department of Water Affairs
DWAF	Department of Water Affairs and Forestry
DWS	Department of Water and Sanitation
ECx	Effect concentrations where x% effect was observed.
EIS	Ecologically Important or Sensitive
ERA	Ecological Risk Analysis
ETMF	Exposure and Toxicity-Modifying Factors
IUA	Integrated Units of Analysis
LCx	Lethal concentrations where x% mortality was observed.
LOEC	Lowest Observed Effect Concentration
MIRAI	Macroinvertebrate Rapid Assessment Index
NOEC	No Observed Effect Concentration
NWA	National Water Act
NWRS	National Water Resource Strategy
PES	Present Ecological State
RDM	Resource Directed Measures
REC	Recommended Ecological Category
RQO	Resource Quality Objective
RU	Resource Units
SARF	Social Amplification of Risk Framework
SAWQG	South African water quality guideline
SDC	Source Directed Controls
SSD	Species Sensitivity Distribution
TWQR	Target Water Quality Range
USEPA	United States Environmental Protection Agency
WER	Water-Effect Ratio

WHO	World Health Organisation
WRC	Water Research Commission

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CHAPTER 1: INTRODUCTION

1.1 INTRODUCTION

All over the world in recent decades, the field of guideline development as a tool for managing freshwater resources has gravitated heavily towards derivation of a risk-based guideline values, which is necessitated by the principle of sustainable development (Vellemu et al., 2018). The current South African water quality guidelines (SAWQGs), while they are easy to use, and have been used widely even beyond South African borders, have been criticised for four fundamental reasons. First, they have been criticised for not being explicitly risk-based and not taking an explicit risk approach in their development and implementation. An important implementation outcome of not being risk-based is what has been refer to as over- or under-protection. In this regard, current guidelines are being used as trigger value, above which an action, usually corrective one, needs to be taken, and below which all is assumed to be fine, and no action may be taken (Heath et al., 2008). However, by taking an explicit risk-based approach in the development and implementation of the revised guidelines, one is forced to ask whether the risk is an acceptable one given management objectives or intended use of the resource. In this sense, an acceptable risk differs between resource protection level, e.g. resource protected at ecological category A, and that protected at ecological category B. This way, the risk-based water quality guidelines take us away from trigger value mind-set that does not reflect different protection levels. By moving towards the risk-based water quality guidelines the decision maker is informed about the consequences of the actions, in terms of its severity, duration and extent, e.g. what proportion of species may die from an event, for how long, and to what extent, and the likelihood of such event occurring. In comparison, a trigger value approach does not necessarily provide such information for management consideration, other than the fact that an action needs to be taken or not.

A second fundamental limitation of the 1996 SAWQGs, that has necessitated the revision exercise, is that they are largely generic, and not site-specific (with the exception of a few variables such as conductivity, pH, total dissolved solids, water temperature) or do not consider the ecological context (Heath, 2008). The underlying principle is that on a spatial level, fundamental contextual differences exist, and therefore, a generic prescriptive value/limit as per the current guidelines, may under protect or over protect depending on the context. Further, water resource users, ecological sensitivity, and importance, also differ spatially, strongly suggesting the criticality of site-specific guidelines, which are not necessarily prescriptive, but indicative of risk to the ecosystem in question at a specified local scale or catchment. Site-specificity implies that the revised guidelines can provide water resource users guidance on identifying, analysing, and managing risk at an appropriate spatial scale, which is currently lacking in the 1996 freshwater ecosystem SAWQGs.

Linked to the first and second limitations is third one, which relates to alignment with the current water resource management strategies. The 1996 guidelines were developed prior to the promulgation of the NWA, as a result, the guidelines do not reflect the thinking informing the various RDM measures. For example, the current guideline for freshwater ecosystems has a single trigger value, which is not very helpful given that the Department of Water and Sanitation (DWS) approach accords water resources different levels of protection, e.g. Class I, II, III and Ecological Categories A-D, with descriptive and quantitative RQOs. An alignment between the guidelines and protection approaches is thus needed, where the probability of effect occurring at a given desired protection level is considered. One of the fundamental implications of aligning the freshwater ecosystem guidelines with current water resource protection approaches is that the guideline needs to be site-specific, in addition to providing risk-based generic measures. The underlying principle is that on a spatial level, fundamental contextual differences exist, and therefore, a generic prescriptive value/limit as per the current guidelines, may under protect or over protect depending on the context. Furthermore, water resources users, ecological sensitivity, and value placed on the resource differ spatially. These clearly underscore the criticality of site-specific guidelines, which are not necessarily prescriptive, but indicative of risk to the aquatic ecosystem in question. Site-specificity implies that the revised guidelines can provide water resource users guidance on identifying, analysing and managing risk at an appropriate spatial scale, which is currently lacking in the 1996 freshwater ecosystem guidelines.

Lastly, since the 1996 guidelines were published, much research has been undertaken locally and internationally in terms of technologies and techniques development, effects of critical pollutants such as pesticides, persistent organic pollutants, endocrine disruptive compounds, pharmaceuticals, and acid mine drainage. Many of these pollutants now considered as being of emerging concerns are not in the current guideline, implying that a revision is urgently needed to reflect new knowledge and research that has been done thus far. This is the fourth reason for the revision of the SAWQGs such that the guidelines include more chemical stressors than the 1996 guidelines.

Guidelines are met among others to support decision making regarding water resource management, as rapidly as possible. In a stakeholder workshop conveyed in 2008, it was agreed that the hard-copy, paper-based guidelines were not fulfilling this purpose, and are cumbersome (Heath et al., 2008). To this end, the water sector stakeholders recommend the development of a software-based decision support system (DSS) flexible enough to allow rapid decision making regarding the risk posed by pollutants of concern. A multi-tier approach is recommended, with an easy to use interface, allowing for easy navigation as well as taking into account DWS capacity and capability as well as existing water quality monitoring networks. It was also recommended that the DSS is updateable, supports educational purpose in addition to decision making, as well as being credible and transparent, with all scientific assumptions, limitations and approaches used fully documented for users to assess. In this regard, the current version of the guidelines is packaged into a user friendly software DSS.

This project largely followed Heath et al. (2008), and Boyd et al. (2015) proposed framework for the revision of risk-based water quality guidelines in South Africa, with some deviations. Thus, the revised South African Water Quality Guideline (SAWQG) for aquatic ecosystems are risk-based, three-tiered approach packaged into a software Decision Support System (DSS).

Tier 1, which represents the scientific domain, is generic and the most conservative guideline, with minimum user input requirement and a simple output provided by the Decision Support System (DSS). This level of guidelines is largely what the 1996 SAWQG details, but has been updated by adding new variables that have become imperatives, as well as updating to current science and in alignment with the Ecological Categories A-F. The Tier 1 guideline is conservative and precautionary in nature as it gives protection to the most sensitive receptor in the aquatic ecosystem. It is also generic due to its applicability to all water resources. Tier 1 guidelines are applicable throughout the country, and should only be used where Tier 2 guidelines do not exist for a particular variable in an ecoregion of interest.

Tier 2 guidelines are ecoregion level II-specific. The ecoregion-specific data are used in the derivation of the guidelines, and are thus more reflective of the environmental context of the specific region. Guidelines at Tier 2 are derived for both water physico-chemistry and macroinvertebrate response. A decision was made to not include fish and riparian vegetation in the guidelines to reduce the complexity as macroinvertebrate alone are known to provide adequate reflection of environmental water quality in freshwater systems. The Department of Water and Sanitation (DWS) data were used in the derivation of the guidelines at Tier 2. As with Tier 1, the DSS generates guidelines outputs aligned with ecological categories A-F.

The Tier 3 guidelines are events/scenario-based. Tier 3 assessment is triggered when unacceptable level of risk is suspected based on the results of Tiers 1 and 2. Tier 3 provides a means for a site-specific water quality risk assessment by collecting detailed site-specific information. A key feature of Tier 3 assessments is that they are event/scenario-based. The reasoning behind this approach is that improving water quality implies a focus on the event/scenario driving water quality change rather than on the symptoms. For the purpose of Tier 3 assessment, risk is conceptualized as a measure of the likelihood (probability) of an event/scenario/issue occurring and its adverse effects or consequence as well as the associated uncertainty. Tier 3 requires highly skilled input and output interpretation. Uncertainties associated with the risk assessment at Tier 3 is also assessed, and the DSS provides a means of doing this.

1.2 PROJECT AIMS

The following were the aims of the project:

8. Review international and national application of risk-based guideline development.
9. Develop a database of spatially referenced data for South Africa, ideally at the quaternary catchment level.
10. Identify requirements for aquatic ecosystem water quality guideline revision.
11. Develop SSD curves for representative taxa exposed stressors selected for guideline revision.
12. Produce and pilot test a software product for aquatic ecosystem water quality guidelines.
13. Finalize aquatic water quality guidelines following user input and with suitable documentation for use.
14. Make recommendations for further research.

1.3 SCOPE AND LIMITATIONS

This technical report on the development of risk-based South African water quality guideline for aquatic ecosystems considered best practices such as application of decision support systems (DSS) and literature review at both the international and local levels. The international literature on risk-based water quality guidelines reviewed included ANZG (2018) for Australia and New Zealand, USEPA (2017) for the United States of America, and CCME (2007) for Canada, while the major South African literature reviewed included DWAF (1996), Warne et al. (2004), Boyd et al. (2015), as well as the National Water Act (Act 36 of 1998). International literature on risk were also reviewed and included: Aven and Renn (2009); Aven and Vinnem (2007); Aven (2010); Aven and Thekdi (2018); Berger et al. (1994); Claassen (1999) and Classen et al. (2001). International and local data were assembled and used for the derivation of risk-based South African water quality guideline. Also, three workshops were also held in the course of the project to solicit inputs of key stakeholders in the water sector. The next chapter deals briefly with the literature review.

CHAPTER 2: LITERATURE REVIEW

2.1 RISK CONCEPTUALISATION

Risk as a concept has been conceptualised differently by different disciplines, resulting in diverse definition of the term. The tradition definition of risk has excessive focus on probability or likelihood (i.e. probabilistic measure of risk). Traditionally, risk has been defined as a measure of the likelihood (probability) of an event occurring and its adverse effects. Risk has also been traditionally conceptualised as the combination of probability of an event and its consequences (Aven, 2010). Risk may also be conceptualised in terms of a "what if scenario". In this case, risk may be viewed as a triplet, i.e. the scenario, the probability of the scenario occurring, and the consequences of the scenario when it does occur (Aven, 2010). A critical reflection of these traditional definitions of risk reveals three important dimensions or indices of risk: (a) the event or scenario, (b) the probabilities (i.e. that of the event occurring and that of the consequence that follows when it does occur), and (c) the consequence (i.e. what would be the outcome when the event does occur). Although severity is often expressed as a dimension of risk, in actual sense, it is a characterisation of the consequence. That is, how severe is the consequence or outcome when the event does occur? These conceptions of risk may be formulated according to Aven (2010) as: ***Risk = (A, C, P)***, where **A** is the event or scenario, **C** is the consequences when A does occur, and **P** is the probabilities associated with **A** and **C**. Using this definition of risk, a risk matrix can be produced as shown in Figure 2.1.

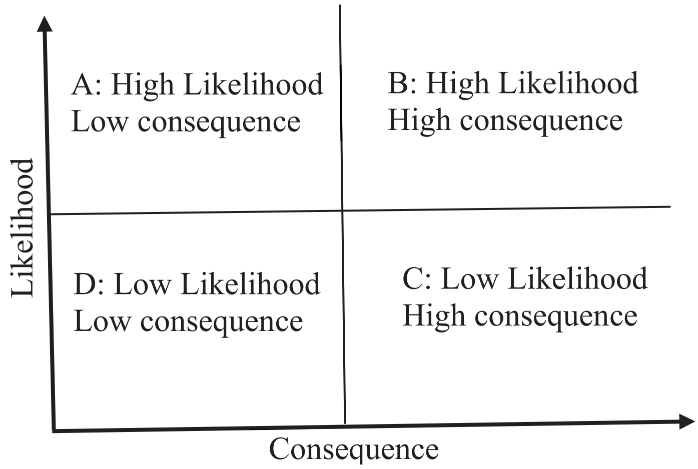

Figure 2.2: Risk matrix based on the likelihood and consequence dimensions of risk

The definition of risk above raised an important fundamental question – that which relates to uncertainty. This is an important question in the expression of risk particularly in the context of ecosystems as inherently complex systems. From the traditional expression of risk, there is an assumption that uncertainty is expressed/captured by the notion of probability/likelihood. Aven (2010) has questioned this assumption, arguing that probabilities alone cannot sufficiently capture uncertainties – whether stochastic or epistemic.

Probability is often interpreted in two main ways: i) the frequentist interpretation and ii) the subjective, knowledge-based interpretation (Berger *et al*., 1994; Cox, 2006; Pek & Van Zandt, 2020) (Bayesian perspective). Regarding the frequentist probability, this relates to relative frequency (*Pf*) (the relative fraction of time) the stressor occurs over a given period. In terms of water quality stressors for example, this can be said to be the relative number of time a concentration of a chemical stressor is above levels where adverse effects can be caused/induced in the receiving environment/receptor (Cox, 2006; Pek & Van Zandt, 2020).

Following this conception of probability, uncertainty is construed as the difference between the “estimated risk” and the true risk, as the actual/true risk is often unknown and is usually estimated (Sutter II, 2006; Pek & Van Zandt, 2020). The uncertainty arising from the frequentist interpretation is often referred to as **stochastic (aleatory) uncertainty**. The second interpretation of probability is that based on the Bayesian perspective. Here, uncertainty is seen as a subjective probability based on the assessor’s background knowledge of the stressor and receptor. It is basically a reflection of the assessor’s belief of the likelihood of the event occurring, and whether if it occurs, the event may or may not induce adverse effects on the receptor or receiving environment. Viewed this way, the subjective probabilities based on the subjective knowledge of the assessor express ***epistemic uncertainty*** – uncertainty about the confidence in how much the assessor knows about the probability of the event occurring and the event causing advance ecological effects. These two kinds of uncertainties have been reflected in the revision of the guidelines (Chapters 3, 4 and 5).

Uncertainty must be seen as an inherent component of risk assessment and risk-based management and decision making. This is particularly true when dealing with complex systems such as freshwater ecosystems and their interaction with and responses to stressors such as chemical pollutants, flow alteration and habitat modification (Carpenter et al., 2011)). In this context, it is thus important that the derivation of the water quality guidelines consider uncertainty, and how uncertainty is accounted for and treated. The treatment of epistemic uncertainty, which reflects the knowledge-based or judgemental dimensions of risk is critical in this regard, particularly at Tiers 2 and 3 in the proposed approach to the derivation of the guidelines. A detailed treatment of how epistemic uncertainty is considered at Tiers 2 and 3.

2.2 REVIEW OF INTERNATIONAL GUIDELINES

2.2.1 Australia and New Zealand

Australian and New Zealand methods for deriving guideline values to protect aquatic ecosystems give consideration to default guideline values (DGVs) and site-specific guideline values (ANZG, 2018). These guideline values for aquatic ecosystems are derived using reference-site data, laboratory-effects data, field-effects data, and multiple lines of evidence, which is based on two or more of these data. Guideline values derived from reference-site data defines a measurable level of change from a natural reference condition that is considered unlikely to result in adverse effects, although the ecological consequences are unknown. For guideline values derived from field and laboratory-effects data, the ecological or biological effects of the stressors are used to define guideline values below which ecologically meaningful changes do not occur.

For chemical and physical lines of evidence, the most preferred data for deriving guideline values is the field and laboratory biological-effects data, followed by local reference data, and then default guideline values (DGVs), which are mostly from the ANZECC & ARMCANZ (2000) Guidelines. The referential approach to deriving guideline value is inherently conservative and a good starting point when no guideline values are available. It is primarily applicable to physical and chemical stressors, but could also be applied to toxicants. Generally, with this approach, guideline values are derived by calculating an appropriate percentile of reference-site data, which often is the 80th percentile. However, more conservative guideline values may be derived as a precautionary measure by applying a lower percentile if there are suspicions that a change from the reference condition could adversely affect ecosystems.

For ecosystem receptors lines of evidence, Water Quality Guidelines include biodiversity, toxicity and biomarkers lines of evidence. Biodiversity lines of evidence could be used to measure the mechanism and extent ecosystems respond to stressors in the environment, and diagnose the nature or identity of the stressor responsible for any measured change to a receptor. Indicators within the biodiversity line of evidence could also serve as early detection and diagnostic tools, and used as direct measures or surrogates of the management goals by giving information on the extent to which ecosystems are being protected or are tracking towards improved ecosystem condition. Any change or departure from a reference condition using biodiversity indicators may represent impact and non-achievement of the management goals. Toxicity and biomarkers lines of evidence could be used as early detection information so that substantial and ecologically important disturbances can be avoided, or diagnostic information in a weight-of-evidence evaluation to detect presence and intensity of responses to stressors (e.g. through direct toxicity assessment) as well as the nature or identity of the stressors eliciting responses. Information obtained from toxicity and biomarkers lines of evidence most often lacks correlation and linkage to effects at higher hierarchy of biological organisation compared to information obtained from indicators within biodiversity lines of evidence. Guideline values for stressors are often based on the effect size associated with a sampling design of specified statistical power to detect any change and/or trend from a reference condition associated with such stressors.

Regional/catchment and site-specific guidelines for physical and chemical stressors

Australia and New Zealand have national, regional/catchment and site-specific guidelines for physical and chemical stressors, as well as for toxicants. Regional guideline values may be derived by applying national guideline values and associated guidance at 80th percentile of reference-site data, or 20th percentile of reference-site data for stressors that cause problems at low concentrations, such as oxygen. Monthly data collected for 2 years sampling at the regional or catchment level are deemed to have adequate ecosystem variability and therefore suitable for deriving guideline values. For high conservation or ecologically important ecosystems, the objective is to keep the water body at the reference condition; for slightly to moderately disturbed ecosystems, test site medians are compared with the 80th percentile guideline values; and for highly disturbed ecosystems, the 90th (or 10th) percentiles are used, with the aim of improving the water quality.

Site-specific guideline values for physical and chemical stressors

Site-specific guideline values are based on monthly monitoring data collected for 2 years from an appropriate site such as un-impacted upstream areas, or from appropriate local reference systems that are representative of unimpacted water bodies. It is advisable that sets of reference sites rather than a single site are used to provide a better characterisation of the local regional characteristics. In regions where water quality is strongly influenced by seasonal or event-scale effects, monitoring data that cover these seasons or events are used to derive guideline values appropriate to the particular period. Where evidence exists that the local ecosystem may be naturally stressed in some seasons (e.g. seasonal depletion of dissolved oxygen), then consideration should be given to the extent by which the ecosystem will be able to accommodate any further move away from median conditions. In these cases, it might be necessary to (i) set the reference-based guideline value at or near the median value, and (ii) ensure that biological monitoring is implemented for assurance of ecosystem protection, as part of a multiple lines-of-evidence approach.

Guideline values for toxicants

Most of the information used to derive toxicant water quality guideline values for Australia and New Zealand is based on laboratory effects data from single-toxicant and single-species toxicity tests. This approach is also used to derive guideline values for chemicals. The toxicant default guideline values (DGVs) in the Water Quality Guidelines are primarily based on literature data mostly derived from standardised tests with commonly used test species in generic laboratory waters. Site-specific guideline values can be derived using species, endpoints and conditions that reflect a specific site or area, provided the methods meet acceptable quality standards.

The methods used to derive the guideline values for both PC stressors and toxicants using laboratory toxicity data are described in “Revised Method for Deriving Australian and New Zealand Water Quality Guideline Values for Toxicants” by Warne et al. (2018), and the “Technical Rationale for Changes to the Method for Deriving Australian and New Zealand Water Quality Guideline Values for Toxicants” by Batley et al. (2018).

Deriving guideline values using multiple lines of evidence

The multiple lines-of-evidence approach to guideline value derivations is thought to ensure greater confidence in the final value in the Water Quality Guidelines. This is because using a mix of field and laboratory data in a multiple lines-of-evidence approach usually provide the best quality of inference in most circumstances. The different datasets from the multiple lines of evidence are evaluated using a weight-of-evidence process. The approach also addresses, to some extent, limitations in conventional toxicity testing methods, including poor ability to characterise certain water quality stressors (e.g. nutrients, suspended sediment, and persistent and bioaccumulative toxicants typically taken up via the diet rather than the water), as well as poor representation of specific groups of species typically found in receiving waters (e.g. aquatic insects) (Cormier et al., 2008; USEPA, 2017). Although the multiple lines-of-evidence approach has many potential applications and guidance on how to use it to derive guideline values, it has not been used to derive default guideline values (DGVs) for Australia and New Zealand. However, it has been suggested that it could be applied in deriving site-specific guideline values where the regulator need to ensure greater confidence in the final value.

2.2.2 United States Environmental Protection Agency

The following review is based on the document entitled “Water Quality Standards Handbook: Chapter 3: Water Quality Criteria” of U.S. Environmental Protection Agency (USEPA) (2017). The USEPA defines water quality criteria as elements of State water quality standards, expressed as constituent concentrations, levels, or narrative statements, representing a quality of water that supports a particular use. When criteria are met, water quality will generally protect the designated use.

The USEPA national criteria are considered generic or default and could be adopted by states and tribes. States and tribes could derive their own criteria with consideration for the national criteria. In that case, the states and tribes water quality criteria must meet three basic requirements: (i) be based on sound scientific rationale, (ii) must contain sufficient parameters or constituents to protect the designated use, and (iii) must support most sensitive designated use of the water body. The USEPA has water quality criteria for human health, recreation, aquatic life, nutrient levels, biological life, flow, sediment, temperature, wildlife, wetlands, priority pollutants, and agriculture and industries.

The USEPA aquatic life water quality criteria

The USEPA Aquatic life water quality criteria (Aquatic Life Guidelines) are useful for protecting aquatic life from the effects of toxic pollutants. They describe an objective method of estimating the highest concentration of a substance in water that will not present a significant risk to the aquatic organisms in the water. This method relies primarily on acute and chronic laboratory toxicity data for aquatic organisms from eight taxonomic groups that reflects the distribution of aquatic organisms’ taxa that are intended to be protected by water quality criteria. Acute criteria are derived using short-term (48-to 96-hour) toxicity tests on aquatic plants and animals. Chronic criteria are derived using long-term (7-day to greater than 28-day) toxicity tests. In the absence of chronic or sufficient chronic data, an acute-to-chronic ratio procedure is used to obtain the desired chronic data. The data are used to derive separate criteria for freshwater and saltwater organisms. Acute and chronic aquatic life criteria may be related to other water quality characteristics such as pH, temperature, or hardness, if justified. Other information from mesocosms (controlled field experiments) and field data are considered when available and as appropriate. This process typically results in numeric criteria but narrative water quality criteria could also be derived using biomonitoring methods where numeric criteria cannot be established or to complement numeric criteria.

The criteria may be expressed as (i) acute to protect against mortality or effects that may result from short-term exposure to toxic substances, and (ii) as chronic to protect against growth and reproductive effects, as well as mortality that may result from a long-term exposure to a chemical. There are three components to both the acute and chronic criteria: criterion magnitude (i.e. the criterion maximum concentration (CMC) for acute criteria and criterion continuous concentration (CCC) for chronic criteria), duration of the CMC and CCC (i.e. averaging period), and a maximum allowable frequency of exceedance of the CMC and CCC. Generally, average durations of one hour for the CMC and four days for the CCC are recommended for aquatic life criteria based on standard laboratory toxicity tests, although there are some exceptions based on unique characteristics of individual pollutants.

Site-specific Aquatic Life Water Quality Criteria

The USEPA guidelines provides that states and authorised tribes may adopt modified water quality criteria that reflect site-specific conditions. A site-specific criterion is developed to protect aquatic life at a particular site, by taking into account a site's physical and chemical conditions. The Site-specific criteria, must be based on a sound scientific rationale, protect designated uses, and are subject to review and approval or otherwise by the USEPA. Site-specific criteria become necessary if the national criteria are deemed under- or over-protective.

The following procedure is recommended by the USEPA for deriving site-specific aquatic life criteria:

(i) A recalculation procedure that takes into account unique differences between the sensitivities of aquatic organisms in the national dataset and the sensitivities of organisms that occur at the site.

(ii) Application of Water-Effect Ratio (WER) procedure that takes into account relevant differences between the toxicities of a metal in laboratory dilution water and in the site water. This procedure applies to metals other than copper.

(iii) Application of biotic ligand model (BLM) that takes into account the effects of all water chemistry parameters that hugely impact copper toxicity, including temperature, pH, dissolved organic carbon, alkalinity, and the presence of specific cations and anions in the water.

2.2.3 Canadian Water Quality Guidelines for the Protection of Aquatic Life

The Canadian Environmental Quality Guidelines (CEQGs) provide science-based goals for the quality of aquatic and terrestrial ecosystems. They include Groundwater Quality Guidelines for Use at Contaminated Sites, Sediment Quality Guidelines for the Protection of Aquatic Life, Soil Quality Guidelines for the Protection of Environmental and Human Health, Soil Vapour Quality Guidelines for the Protection of Human Exposure Via Inhalation of Vapours, Tissue Residue Guidelines for the Protection of Wildlife Consumers of Aquatic Biota, Water Quality Guidelines for the Protection of Agricultural Water Uses, and Water Quality Guidelines for the Protection of Aquatic Life. The Canadian Water Quality Guidelines for the Protection of Aquatic Life (CWQGs-PAL) are useful for protecting all forms of aquatic life and all aspects of aquatic life cycles, including the most sensitive life stages of the most sensitive species over the long term from anthropogenic stressors such as chemical inputs or changes to physical components. They provide science-based benchmarks for a nationally consistent level of protection for aquatic life.

The original protocol for deriving CWQGs-PAL was published in 1991 and the current version was published in 2007. This review is based on the current protocol entitled "A Protocol for the Derivation of Water Quality Guidelines for the Protection of Aquatic Life 2007", which is referenced in-text as CCME (2007). The protocol makes explicit guideline derivation for long-term and short-term exposure periods, and recommends two derivation approaches depending on type of data available.

Site-specific and national guidelines

Site-specific guidelines are derived taking into consideration the natural background concentration of naturally occurring substances, and therefore, cannot be incorporated into a nationally applicable guideline value. The data used for site-specific guidelines are from location-dependent toxicological studies. The national guideline is derived considering all acceptable and applicable toxicological data from a variety of toxicological studies, which were performed with different species, with different histories, and under different exposure conditions. Using these location-independent toxicological studies could result in the recommended national guideline value falling below (or outside) the natural background concentration (or natural condition) of a particular site of interest. It is recommended that the natural background concentrations should be taken as the site-specific guideline value where the natural background concentration of a substance exceeds the national guideline value derived primarily from laboratory toxicity data. However, another appropriate site-specific guideline value may be derived according to recommended methods (e.g. CCME, 2007).

Short-term and Long-term guidelines

The protocol (CCME, 2007) makes provision for deriving both short-term and long-term exposures guidelines. Short-term exposure guidelines identify benchmarks (i.e. maximum concentrations of substances or ranges for attributes) in the aquatic ecosystem that protect only a specified fraction of individuals from severe effects like mortality for a defined short-term exposure period. By definition and design, short-term guidelines do not fulfil the guiding principle of protecting all components of the aquatic ecosystem all the time. Long-term exposure guidelines identify benchmarks (i.e. maximum concentrations of substances or ranges for attributes) in the aquatic ecosystem that are intended to protect all forms of aquatic life (all species, all life stages) for indefinite exposure periods. The impacts of exposure and toxicity-modifying factors (ETMFs) such as pH, temperature, hardness (Ca2+, Mg2+), organic matter, oxygen, and other physicochemical substances are incorporated into the derivation of guidelines, provided that the scientific information to do so is available.

Total and bioavailability guidelines

The protocol recommends two guidelines (total and bioavailable) values for substances that exhibit a complex environmental chemistry and toxicology (e.g. metals), thereby creating unique challenges in their guideline derivation and environmental management. Total guideline value is based on the total measured concentration in the unfiltered sample (i.e. total recoverable concentration). It does not factor in bioavailability and is, thus, highly conservative. The bioavailability guideline is based on the relevant physical and chemical speciation-specific fractions (i.e. the fractions toxic to aquatic organisms). This guideline factors in bioavailability and is, thus, more realistic. The bioavailability guidelines focus on the potentially toxic forms of substances due to their bioavailability.

Type A and Type B guidelines

The protocol for deriving guidelines values (CCME, 2007) makes provision for two approaches to derive water quality guidelines, depending on the availability and quality of data for the substance. Each approach requires a defined minimum amount of environmental and toxicological data. Type A guidelines, which are the more preferred, are based on the statistical distribution of all the available and acceptable toxicity data. They are derived using a species sensitivity distribution (SSD) approach when there are adequate primary and secondary toxicity data to satisfactorily fit an SSD curve. Type B guidelines are based on the extrapolation from the lowest available and acceptable toxicity endpoint. They are derived for substances that either have inadequate or insufficient toxicity data for the SSD approach, but for which enough toxicity data from a minimum number of primary and/or secondary studies are available. Type B guidelines are sub-divided into Type B1 and Type B2 guidelines, based on the quantity and quality of available toxicity data. At present, there is no protocol for deriving guidelines when the minimum toxicity data requirement for a Type B guideline is not met.

The recommended guideline derivation method involves modelling the cumulative species sensitivity distribution (SSD) with estimating the 95% confidence interval. The guideline is defined as the intercept of the 5th percentile of the SSD. The short-term exposure guideline is extrapolated from severe-effects threshold data, while the long-term exposure guideline is extrapolated primarily and preferentially from no-effect threshold data. The preferred endpoint for deriving long-term exposure guidelines is the most appropriate acceptable long-term exposure ECx of a standard test. Other tests are acceptable if the ECx value has been derived by regression analysis of the toxicological data and it has been demonstrated to be at or near the no-effects threshold. If the quantity of no-effect ECx threshold data are not sufficient to meet the minimum data requirement, then less preferred endpoints may be added to the dataset sequentially in the following order: most appropriate ECx/ICx representing a no-effects threshold > EC10/IC10 > EC11-25/IC11-25 > MATC > NOEC > LOEC> nonlethal EC26-49/IC26-49 > nonlethal EC50/IC50.

CHAPTER 3: SOUTH AFRICAN WATER QUALITY GUIDELINES FOR FRESHWATER ECOSYSTEMS: VERSION 2 – TIER 1

3.1 INTRODUCTION

The 1996 aquatic ecosystem guidelines, the last that were produced, were based on toxicological studies, supplemented by other input from other standards, and expert consultation (DWAF, 1996, Roux et al., 1996). The guidelines themselves gave different levels of potential toxicants to conform to a Target Water Quality Range (TWQR), Chronic Effect Value and Acute Effect Value. These were derived using methods outlined in DWAF (1996) and Roux et al. (1996), largely following USEPA methods described by Stephan et al. (1985). The Acute Effect Value is a concentration of the toxicant at and above which significant adverse acute impacts are expected (Roux et al., 1996). The Chronic Effect Value is the concentration at which all or most populations would be safe during continuous exposure (Roux et al., 1996). The Target Water Quality Range is a management objective that specifies an ideal concentration range of a particular compound (DWAF, 1996). These levels are not formally related to other management tools such as Ecological Categories, Fitness for Use Categories, Management Classes, etc.

The use of toxicological results in setting of guidelines has wide application (e.g. Warne et al., 2018, Suter, 2002, Van Straalen and Van Leeuwen, 2002). It is a method that appeals in its directness and simplicity. Determining the response of a taxon to a compound is a straightforward way to identify levels of that compound that would have limited impact on that taxon. Expanding to the use of multiple species to account for the variation in toxicological response between taxa is a logical extension of simple toxicological testing (Van Straalen and Van Leeuwen, 2002). If a wide enough range of taxa are assessed, they may approximate the response of communities in the field. This is where Species Sensitivity Distributions (SSDs) have a role.

Taxa in rivers have a range of ecologies, physiologies, morphologies, and behaviours. These differences mean that different species have different sensitivities to any specific compound. SSDs attempt to fit that variation to a statistical distribution to allow interpolation and to use the model to predict community responses. The fitted model can form the basis for guideline derivation and Ecological Risk Analysis (e.g. Posthuma et al., 2019, Solomon and Takacs, 2002, Traas et al., 2002, Warren-Hicks et al., 2002).

Despite their wide application in setting water quality guidelines, SSDs are also limited as a tool that predicts community level responses to particular compounds. SSDs generally treat a single compound, or related compounds, while a natural community can be exposed to mixtures of compounds and methods are needed for these circumstances (de Zwart and Posthuma, 2005, Belanger et al., 2017, Brack et al., 2019). SSDs do not consider food-chain exposure or other taxon-mediated community effect (Posthuma et al., 2019). Finally, a good prediction of a community response relies on adequate and appropriate taxon representation in the SSD model, and these data may be lacking (Posthuma et al., 2019).

2.2 METHODOLOGY

Posthuma et al. (2019) demonstrated the utility of using Species Sensitivity Distributions (SSDs) to produce a range of guideline values for compounds. Their study noted that SSDs had been applied in the past under strict data criteria, or where taxonomic diversity criteria had been strict and as a result the SSD analyses were based on limited records, and hence with potentially limited statistical power. In contrast they tested an approach that aimed to produce chemical-specific SSDs, and for each chemical, to produce an acute and chronic SSD, with a matching quality score. In doing so, they combined results from different tests, as long as certain criteria were met.

3.2.1 Data

Data sources were selected following Posthuma et al. (2019), who generated protective guidelines for more than 12 000 chemicals from publicly available data sets. Only the larger datasets they describe were used as the smaller datasets had relatively few records.

Toxicological data were downloaded from the USEPA Ecotox database (Olker et al., 2022) in May 2021. Text files with received data were uploaded to PostgreSQL database, and compiled to a single table. Data were simplified as required, and filtered such that only valid freshwater ecotoxicological records were used, giving a final data set of 165 320 valid freshwater toxicology records on 907 compounds.

The other primary source of data was MistraPharma's WikiPharma database (Molander et al., 2009), downloaded in January 2022. This data source contains the results of toxicological testing for environmental effects of pharmaceuticals in freshwater. WikiPharma contains 7 999 toxicological endpoint records of 341 compounds.

All data were compiled together in a database, and formats were standardized where necessary. WikiPharma records, which on receipt had multiple endpoints per record, were modified to give one endpoint per record. WikiPharma records had a CAS Registry Number assigned where the compound was to be included in the guidelines. The CAS Registry Number provides a unique identification number from the Chemical Abstracts Service (CAS) to every chemical substance described in the open scientific literature (CAS 2023). As chemical naming conventions may vary, the CAS number is useful as a means of identifying compounds in the database. WikiPharma did supply an ATC code for each compound. The Anatomical Therapeutic Chemical (ATC) code is a unique code assigned by the World Health Organization (WHO) to a medicine according to the organ or system it works on and how it works (WHO 2023). The ATC codes are not compound-specific, and so, for data management, it was replaced by the CAS Number in the database. Finally, the units for concentrations of compounds assessed were standardised to mg/ℓ.

3.2.2 Compounds assessed

The compounds selected to be included in the guideline are presented in Table 3-1. They are separated for convenience into three groups: inorganic compounds; organic compounds; and pharmaceuticals.

For most organic compounds and pharmaceuticals, using toxicological data to derive a guideline is fairly straightforward, as toxicological tests are run on the dissolved compounds directly. Inorganic compounds, which are usually tested in the form of one or another salt, are more complex, as the toxicological results reflect the combined impact of ions on the test organism(s). However, management systems utilise measures of the active compound, and not its salt, and so guidelines for individual compounds or elements are required.

Table 3-1 Compounds included in the Tier 1 guidelines

Inorganic	Organic	Pharmaceuticals
Aluminium	1-Chloronaphthalene	Acetylsalicylic acid
Ammonia	1,2,3,7,8-Pentachlorodibenzo-P-dioxin	Amoxicillin
Arsenic	2-Chloronaphthalene	Ampicillin
Boron	2,3,7,8-Tetrachlorodibenzo-p-dioxin	Azithromycin
Cadmium	2,4-D	Chloramphenicol
Chlorine	Aniline	Chloroquine
Chromium	Anthracene	Ciprofloxacin
Cobalt	Atrazine	Diclofenac
Cyanide	Benzene	Erythromycin
Copper	Biphenyl	Estradiol
Fluoride	Carbaryl	Estriol
Iron	Chlorobenzene	Estrone
Lead	Chlorophenols	Ethinylestradiol
Lithium	Chlorpyrifos	Hydrochlorothiazide
Manganese	Cypermethrin	Ibuprofen
Mercury	DDT	Lidocaine
Nickel	Deltamethrin	Metronidazole
Selenium	Dicofol	Ofloxacin
Silver	Dieldrin	Paracetamol
Tin	Diquat	Propranolol
Uranium	Endosulfan	Salicylic acid
Vanadium	Endrin	Streptomycin
Zinc	Ethanol	Sulfadiazine
	Ethylbenzene	Sulfamethoxazole
	Flourene	Testosterone
	Glyphosate	Tetracycline
	Heptachlor	
	Imidacloprid	
	Isopropanol	
	Lindane	
	Malathion	
	Naphthalene	
	Nitrobenzenes	
	Paraquat	
	Parathion	
	Phenalene	
	Phenanthrene	
	Phenol	
	Polychlorinated biphenyls	
	Pyrene	
	Toluene	
	Tributyltin	
	Xylene	

In order that guidelines on inorganic ions could be included, salts were identified where the compound being tested was assessed using several of its salts. These were selected in order that the toxicological impact of the associated ion would not be high and therefore that the toxicological response would indicate to a great extent the compounds or elements being tested. What this in effect meant was that, for any given cation, the chloride, sulphate, hydroxide and carbonate salt results were used together to determine the SSD. For anions, the hydrogen, sodium, potassium, and magnesium salts would be considered. Different hydration states of the salts were also combined. In all cases, as the effect concentrations were measured in mg/ℓ, the effect concentration needed to be modified by the mass fraction, a factor that indicated what mass of the compound in question was that compound itself, and what was due to other components of the salt. Selection of ions assessed inorganic, organic and pharmaceutical tables was based on what toxicological data are available, and not what salts or compounds might be possible in theory. Likewise, naming conventions followed toxicological database records standards. The salts or other compounds used to generate SSDs in this way are given in Table 3-2.

Table 3-2 List of salts or compounds that were used to generate SSD curves for compounds of elements where simple direct toxicological data were limited or not available.

Compound/Element	Salt/Linked Compound	Other specification
Aluminium	Aluminium	
	Aluminium chloride	Anhydous
	Aluminium hydroxide	
	Aluminium sulfate	
Ammonia	Ammonia	
	Ammonia solution	
Arsenic	Arsenic	
	Arsenic trichloride	
	Arsenous acid	
Boron	Boric acid, Barium salt	
	Boron	
Cadmium	Cadmium	
	Cadmium carbonate	
	Cadmium chloride	
	Cadmium sulfate	Anhydous
	Cadmium sulfate	Octahydrate
Chlorine	Chlorine	
Chromium	Chromium	
	Chromium (III) carbonate	
	Chromium (II) chloride	Anhydrous
	Chromium (II) sulfate	Anhydrous
	Chromium (II) sulfate	Pentahydrate
	Chromium (II) sulfate	Trihydrate
	Chromium (III) chloride	Anhydrous
	Chromium (III) chloride	Hexahydrate
	Chromium (III) hydroxide	Anhydrous
	Chromium (III) hydroxide	Dihydrate
	Chromium (III) sulfate	Anhydrous
	Chromium (IV) chloride	
Cobalt	Carbonic acid, Cobalt salt	
	Cobalt	
	Cobalt (II) chloride ($CoCl_2$)	Anhydrous
	Cobalt (II) chloride ($CoCl_2$)	Dihydrate
	Cobalt (II) chloride ($CoCl_2$)	Hexahydrate
	Cobalt (II) sulfate	Anhydrous
	Cobalt (II) sulfate	Heptahydrate
	Cobalt (II) sulfate	Hexahydrate
	Cobalt (II) sulfate	Monohydrate

Compound/Element	Salt/Linked Compound	Other specification
	Cobalt (III) chloride ($CoCl_3$)	
	Nitric acid, Cobalt (2+) salt (2:1)	
Copper	Copper	
	Copper (I) chloride	
	Copper (I) hydroxide	
	Copper (II) carbonate	
	Copper (II) chloride	Anhydrous
	Copper (II) chloride	Dihydrate
	Copper (II) hydroxide	
	Copper (II) sulfate	Anhydrous
	Copper (II) sulfate	Heptahydrate
	Copper (II) sulfate	Pentahydrate
	Copper (II) sulfate	Trihydrate
Cyanide	Hydrogen cyanide	
	Potassium cyanide	
	Sodium cyanide	
Diquat	Diquat dibromide	
	Diquat dichloride	
Fluoride	Calcium fluoride	
	Fluoride	
	Magnesium fluoride	
	Potassium fluoride	Anhydrous
	Potassium fluoride	Dihydrate
	Sodium fluoride	
Iron	Iron	
	Iron (II) hydroxide	
	Iron (II) carbonate	
	Iron (II) chloride	Anhydrous
	Iron (II) chloride	Dihydrate
	Iron (II) chloride	Tetrahydrate
	Iron (II) sulfate	Anhydrous
	Iron (II) sulfate	Dihydrate
	Iron (II) sulfate	Heptahydrate
	Iron (II) sulfate	Monohydrate
	Iron (III) chloride	Anhydrous
	Iron (III) chloride	Dihydrate
	Iron (III) chloride	Hexahydrate
	Iron (III) oxide-hydroxide	
	Iron (III) sulfate	Anhydrous
	Iron (III) sulfate	Monohydrate
Lead	Lead	
	Lead (II) carbonate	
	Lead carbonate hydroxide	
	Lead (II) chloride	
	Lead (II) hydroxide	
	Lead (II) sulfate	
	Lead (IV) chloride	
	Lead (IV) hydroxide	
Lithium	Lithium carbonate	
	Lithium citrate	

Compound/Element	Salt/Linked Compound	Other specification
Manganese	Manganese	
	Manganese hydroxide oxide	
	Manganese (II) carbonate	
	Manganese (II) chloride	Anhydrous
	Manganese (II) chloride	Dihydrate
	Manganese (II) chloride	Tetrahydrate
	Manganese (II) hydroxide	
	Manganese (II) sulfate	Monohydrate
	Manganese (II) sulfate	Tetrahydrate
	Manganese (II) sulfate	Anhydrous
Mercury	Mercury	
	Mercury (I) carbonate	
	Mercury (I) chloride	
	Mercury (I) sulfate	
	Mercury (II) chloride	
	Mercury (II) hydroxide	
	Mercury (II) sulfate	
Nickel	Nickel	
	Nickel chloride	Hexahydrate
	Nickel chloride ($NiCl_2$)	Anhydrous
	Nitric acid, Nickel (2+) salt (2:1)	
	Sulfuric acid, Nickel (2+) salt (1:1)	Anhydrous
	Sulfuric acid, Nickel (2+) salt (1:1)	Heptahydrate
	Sulfuric acid, Nickel (2+) salt (1:1)	Hexahydrate
Paraquat	Paraquat dichloride	
	Paraquat diiodide	
	Paraquat methosulphate	
Selenium	Potassium selenite	
	Potassium selenite	
	Selenic acid	
	Selenic acid, sodium salt (1:2)	
	Selenious acid	
	Selenious acid, disodium salt	Pentahydrate
	Selenious acid, monosodium salt	
	Selenious acid, sodium salt	
	Selenious acid, sodium salt (1:2)	
	Selenium	
	Selenium dichloride	
	Selenium disulphide	
	Selenium monochloride	
	Selenium oxide (SeO_2)	
	Selenium tetrachloride	
	Sodium selenide (Na_2Se)	
Silver	Nitric acid silver (1+) salt (1:1)	
	Silver	
	Silver chloride	
	Silver sulfate	
	Silver (1+) sulfide	
	Thiosulfuric acid, disilver (1+) salt	
Tin	Tin	

Compound/Element	Salt/Linked Compound	Other specification
	Tin chloride ($SnCl_2$)	
Tributyltin (TBT)	Tributyltin (TBT)	
	Tributyltin 2-pyridinecarboxylate	
	Tributyltin 3-pyridine carboxylate	
	Tributyltin methanesulphonate	
Uranium	Uranium	
Vanadium	Oxo [sulfato (2-)-o] vanadium	
	Sodium vanadium oxide (Na_3VO_4)	
	Vanadium	
	Vanadium oxide (V_2O_5)	
Zinc	Zinc	
	Zinc carbonate	
	Zinc carbonate hydroxide	
	Zinc chloride	Anhydrous
	Zinc chloride	Tetrahydrate
	Zinc hydrogen carbonate	
	Zinc hydroxide	
	Zinc sulphate	Anhydrous
	Zinc sulphate	Heptahydrate
	Zinc sulphate	Hexahydrate
	Zinc sulphate	Monohydrate

3.2.3: Endpoints

The datasets that underlie these Tier 1 guidelines had diverse endpoints, and in order to proceed to SSD analysis to produce a guideline it is necessary to refine the datasets to one appropriate for the compound in question. A decision was made to expand the size of compound-specific datasets by lightly relaxing endpoint selection criteria slightly such that similar data on the compound in question could contribute to the dataset passed for analysis. This approach was adopted to increase data available and so maximise the number of compounds for which guidelines are returned. Dataset size has been identified as of concern as SSDs derived from small or skewed datasets lead to lowered confidence in the model and hence any derived guidelines (Wheeler et al., 2002, Kamo, 2023). In expanding the dataset in this way, the methods selected for Tier 1 follow Posthuma et al. (2019) to a certain extent.

Generally, toxicity can either be classified as acute or chronic. Here, these follow general conventions (e.g. Batley et al., 2018; EPA 2023) and in the context of the project are defined as:

- Acute: Acute tests are short-term exposure tests to a potential toxicant. They commonly have lethality as an endpoint. For this guideline, data selected are those from tests that assess mortality and that return valid numeric endpoints that assess impacts on 40-60% of the population (the great majority of these data were labelled as EC_{50} or LC_{50}).

- Chronic: Chronic tests are longer term exposures to potential toxicants. They generally use a sublethal endpoint that assesses a criterion relevant to the test population. Here, data selected are those from tests that affect growth, development, reproduction, physiology, genetics, and behaviour and feeding of the test taxa and that returned valid numeric data for NOEC, LOEC and other endpoints returning data for effects that impact 10% or less of a population.

3.2.4 Implementation

Once appropriate records on toxicity test results are selected, they were transmitted to R (R core team 2022), where they undergo a Species Sensitivity Distribution (SSD) analysis using the ssdtools package (Thorley and Schwarz, 2018). SSDs are recognised as a means of utilizing ecological risk-based methods in guideline derivation (Posthuma et al., 2002b). Risk assessment using SSDs assesses one possible undesired event, the exposure of an arbitrarily chosen species to an environmental concentration greater than its no-effect level (Van Straalen, 2002).

Derived acute or chronic datasets for the compound being assessed are loaded to ssdtools, where log logistic, gamma and log normal distributions are fitted to the data. The final model fit is derived from a model averaging procedure using Akaike Information Criteria. Finally, a parametric bootstrap (1000 repetitions) is used to generate confidence intervals on the hazard concentrations.

These data can then be used to estimate what proportion of aquatic taxa might be threatened by a given concentration of a particular toxicant. The nature of the potential threat will depend on what endpoints are assessed. In particular, endpoints like EC_{50} or LC_{50}, which assess the effect at median population impacts, would be different to NOEC/LOEC/EC_5 endpoints, which assess the concentration at which the compound has no or little impact on the test taxon. Likewise, tests that assess mortality as a response are different to tests assessing, for example, behaviour.

3.2.5 Ecological Categories

The SSD analyses are used to generate guidelines for each compound from the final SSD model fit (see Table 3-3). The guidelines for each Ecological Category will protect the taxa as presented. The lower the guideline value, the greater the hazard presented. Each guideline value will be accompanied by an indication of the confidence in the presented guideline.

Table 3-3 Guideline derivation for application to SSD consensus model fits. Corresponding to generic ecological categories of Kleynhans and Louw (2007). NB x, is the guideline value at a given ecological category, and +y is the upper predicted confidence interval, and -y is the lower predicted confidence interval.

Ecological Category	Name	QW Guideline value	Description
A	Natural	x ±y	Concentration of a water quality constituent most likely suitable for 99% of species. The risk of more than 1% of species being affected is low. Extremely sensitive species may still be affected.
B	Largely natural	x ±y	Concentration of a water quality constituent most likely suitable for 95% of species. The risk of more than 5% of species being affected is low. Highly sensitive species may still be affected.
C	Moderate impact	x ±y	Concentration of a water quality constituent may affect considerable number of species. The risk of at least 10% of the species being affected is high, with moderate impact on biodiversity and ecosystem functionality.
D	Large impact	x ±y	Concentration of a water quality constituent may affect huge number of species. The risk of at least 20% of the species being affected is high, with large impact on biodiversity and ecosystem functionality
E	Serious impact	x ±y	Concentration of a water quality constituent may affect huge number of species. The risk of at least 30% of the species being affected is serious, with serious impact on biodiversity and ecosystem functionality. Water quality is unacceptable.
F	Critical impact	x ±y	Concentration of a water quality constituent may affect huge number of species. The risk of at least 40% of the species being affected is critical. Water quality is unacceptable.

3.2.6 Tier 1 Guidelines

Tier 1 Guidelines are thus read from the SSD curve corresponding to a particular protection level as indicated in Table 3-3.

CHAPTER 4: SOUTH AFRICAN WATER QUALITY GUIDELINES FOR FRESHWATER ECOSYSTEM: VERSION 2 – TIER 2

4.1 INTRODUCTION

South Africa rivers are spatially variable and heterogenous. This spatial variability is driven by several factors such as climate, physiography, geology and soils as well as attitude. As a result, rivers in South Africa have been typed hierarchically into ecoregion levels I and II. The underlying assumption is that rivers within the same ecoregion are ecologically more similar than rivers in distinct ecoregions. One of the criticisms of the 1996 Guidelines is that they were prescriptive without taking spatial variability into account in the sense that the same guideline values were applied throughout the country. A key short-coming of this approach is that in some parts of the country, certain water quality variables are naturally elevated due to underlying natural factors, e.g. some coastal rivers in the Eastern Cape such as Swartkops River that has elevated salt levels due to the underlying geology. The revised guidelines accounted for spatial variability within the country by deriving guidelines at ecoregion level II, and using site-specific information to assess risk posed to ecosystems at Tier 3 (see next chapter).

4.2 DERIVATION OF PHYSICO-CHEMICAL GUIDELINES AT TIER 2

Tier 2 Guidelines were derived using the DWS data in the WMS database. WMS maintains a good set of data on major salts and other commonly measured physico-chemical variables such as nutrients, pH and dissolved oxygen, but has very little data on organic contaminants including herbicide and pesticide levels (guidelines for organic chemicals were derived at Tier 1 using toxicological data). WMS contains data from 333 routinely monitored points, which were relied upon as the primary source of data for the derivation of Tier 2 Guidelines. These data cover the period 1970s-2020 but this varies by ecoregion. The DWS data covers all seasons in South Africa, and by using these spatially and seasonally variable dataset, the revised guidelines thus account for both spatial and seasonal variability. Given the general rarity of data on metals in WMS, and the near absence of data on organic toxins, guidelines for these variables were derived only at Tier 1 based on ecotoxicological data, and may be regarded as conservatives.

Tier 2 physico-chemical guidelines were derived at ecoregion level 2. The DWS data were processed and regionalised. The derivation of the guidelines follows mainly the water quality methods for the Reserve (DWAF 2008), with some modifications. The Reserve method places emphasis on the use of data from over earliest three-year period, but an exploration of the data per ecoregion level II suggests data paucity in many of the ecoregions. Therefore, the guidelines were developed based on all data reported for an ecoregion. For nutrients and common inorganic salts, the guidelines were developed as per Table 4-1 using DWS data.

The confidence level associated with each ecoregion level 2 guideline values were determined on the basis of the number of samples/data points used in the guideline derivation as shown in Table 4-2. The confidence values are returned by the Decision Support System (DSS) with the guideline values. Interpretation of results must thus give credence to the associated confidence level to each guideline value at ecoregion level 2.

Table 4-1 Guideline values for nutrients and common salts at ecoregion level 2, corresponding to generic ecological categories of Kleynhans and Louw (2007).

Ecological Category	Name	Guideline values	Description
A	Natural	5th percentile	Unmodified and natural condition
B	Largely natural	15th percentile	Largely natural with small change from reference conditions.
C	Moderate impact	40th percentile	Moderate change from reference concentrations.
D	Large impact	60th percentile	Large change from reference conditions
E	Serious impact	80th percentile	Serious and extensive change from reference conditions. Condition is unacceptable.
F	Critical impact	95th percentile	Critical and extreme change to ecosystems. Condition is unacceptable.

Table 4-2 Confidence level associated with ecoregion level 2 guideline values.

Confidence	Description
High	A minimum of 60 samples were used in the derivation of the guideline values.
Moderate	A minimum of 25 samples were used in the derivation of the guideline value
Low	A minimum of 12 samples were used in the derivation of the guideline value

The methodology for dissolved oxygen recognises that this is a parameter that varies over each day, as a result of changes of photosynthetic oxygen production and other metabolic processes (e.g. Riley and Dodds, 2013). For this reason, ecoregion level 2 records of oxygen levels are of little use in guideline production, as there is little control over sampling time. In addition, the number of records is limited.

As a result, the following methods are recommended for assessing dissolved oxygen levels at any particular site. Sample water from just below the surface of the water body. Either collect the sample at 06h00, when dissolved oxygen levels can be expected to be low. Alternately, use the lowest instantaneous concentration recorded in a 24-hour period. The oxygen needs to be measured as soon as possible after collection, ideally on site to ensure that sample oxygen levels do not change. If the sample is to be stored for a short period, ensure that there is no air in the sample container, and store the sample in the dark at 4°C, and measure oxygen levels before in-sample metabolism is able to significantly change the level of oxygen present.

The solubility of oxygen in water varies with temperature. Therefore, the guidelines present different recommendations for differing temperatures. Guidelines are presented as both oxygen concentrations and percentage oxygen saturation (Table 4-3).

Table 4-3 Guideline values for dissolved oxygen at a range of different temperatures in freshwater.

	Name	Guideline values	Description
A	Natural	120-100% or 9.91-8.26 mg/L (at 25°C) 120-100% or 10.91-9.10 mg/L (at 20°C) 120-100% or 12.11-10.09 mg/L (at 15°C)	Unmodified and natural condition
B	Largely natural	<100-80% or <8.26-6.61 mg/L (at 25°C) <100-80% or <9.10-7.28 mg/L (at 20°C) <100-80% or <10.09-8.07 mg/L (at 15°C)	Largely natural with small change from reference conditions.
C	Moderate impact	<80-60% or <6.61-4.96 mg/L (at 25°C) <80-60% or <7.28-5.46 mg/L (at 20°C) <80-60% or <8.07-6.05 mg/L (at 15°C)	Moderate change from reference concentrations.
D	Large impact	<60-40% or <4.96-3.30 mg/L (at 25°C) <60-40% or <5.46-3.64 mg/L (at 20°C) <60-40% or <6.05-4.04 mg/L (at 15°C)	Large change from reference conditions
E	Serious impact	<40-20% or <3.30-1.65 mg/L (at 25°C) <40-20% or <3.64-1.82 mg/L (at 20°C) <40-20% or <4.04-2.02 mg/L (at 15°C)	Serious and extensive change from reference conditions. Condition is unacceptable.
F	Critical impact	<20% or <1.65 mg/L (at 25°C) <20% or <1.82 mg/L (at 20°C) <20% or <2.02 mg/L (at 15°C)	Critical and extreme change to ecosystems. Condition is unacceptable.

The method for deriving pH guidelines takes into account the natural spatial variability the occurs as pH is affected by geographic and geological differences and longitudinal differences. The method also reflects whether the background pH is acidic or alkaline as well as the influences of temporal variability due to diel differences and seasonal differences. pH guidelines were derived using the earliest three-year data (post-1990) in ecoregion level II (Table 4-4). The earliest three-year post-1990 data were used because of the anomaly which had been detected in the pre-1990 data of the WMS database for pH (Ramjukadh et al., 2018).

Table 4-4: Guideline values for pH at ecoregion level 2, corresponding to generic ecological categories of Kleynhans and Louw (2007).

Ecological Category	Name	Guideline values	Description
A	Natural	45-55th percentile	Unmodified and natural condition
B	Largely natural	37-45th percentile (acidic) 55-63rd percentile (basic)	Largely natural with small change from reference conditions.
C	Moderate impact	29-37th percentile (acidic) 63-71st percentile (basic)	Moderate change from reference concentrations.
D	Large impact	21-29th percentile (acidic) 71-79th percentile (basic)	Large change from reference conditions
E	Serious impact	13-21st percentile (acidic) 79-87th percentile (basic)	Serious and extensive change from reference conditions. Condition is unacceptable.
F	Critical impact	<13th percentile (acidic) >87th percentile (basic)	Critical and extreme change to ecosystems. Condition is unacceptable.

An exception to the above approach occurs when a user requests guidelines for temperature. Comprehensive methods for producing freshwater temperature guidelines have been produced by Dallas and Rivers-Moore (2019a, 2019b, 2022), and the user is directed to their work.

In Summary, Dallas et al. (2019b) recommends a two-step approach for water temperature. First, a Screening Process is undertaken, where the practitioners determine whether or not water temperature should be considered at a particular site, be it for setting an environmental water temperature guideline or evaluating the potential effect of a thermal impact. Aspects such as site, reach or river resilience, hydrological and water quality factors, and sensitivity of river organisms, are considered. An assessment of thermal stress in terms of risk forms the final stage of the screening process. If risk is deemed to be Moderate, high or very high, then the second step is undertaken. Step 2, the This Evaluation Process, includes two components: a) Establishing Reference Indicators of Thermal Alteration (thermal metrics) and a Reference Thermograph, and b) Evaluating deviation from Reference thermal metrics and a Reference Thermograph.

4.3 MACROINVERTEBRATE RISK MODEL

In addition to physico-chemical constituents, Tier 2 guidelines also uses macroinvertebrate biomonitoring data. The expected assemblage per ecoregion level 2 were derived from the Macroinvertebrate Response Assessment Index (MIRAI) model version 2 (Thirion, 2007). The rationale is that under reference conditions, the expected assemblage should be similar to those observed. To derive macroinvertebrate-based guidelines at Tier 2, a macroinvertebrate risk model was developed and implemented. The macroinvertebrate risk model relies on three metrics: ecoregion level 2 presence and associated confidence, geozone presence and associated confidence and water quality sensitivity.

The ecoregions are spatial areas defined by terrain and vegetation, with similar altitude, rainfall, runoff variability, air temperature, geology and soil. They follow the ecoregional typing approach developed by Omernik (1987). Level 2 ecoregions underlie the reference taxa generation method employed by MIRAI V2, and are used for this purpose in the macroinvertebrate risk model. MIRAI provides an estimation of the confidence of a given macroinvertebrate taxon occurring in a particular ecoregion level 2. These ecoregional presence confidence levels are 1, 3 and 5, where 5 indicates the highest confidence level implying the highest assurance that the taxon does occur in the region, whereas 1 implies a very low confidence that the taxon does occur in the region, whereas 3 is a moderate confidence level regarding the taxon occurrence within the ecoregion level 2. Based on the ecoregional presence data, an impact on the macroinvertebrate assemblage is implied to have occurred: 1) if an expected taxon in the region was not observed; 2) if an unexpected taxon within the region was observed. The presence of an expected taxon in the observed data implies no impact or risk. The relationship between presence confidence weighting and risk to the resource as conceptualised in the macroinvertebrate risk model is shown in Table 4-5.

The longitudinal zonation of rivers in South Africa provides a system of classifying rivers down the channel length according to key gemmological features such as gradient, bed materials, flow and hydraulic characteristics (Rowntree et al., 2000). These features regulate the occurrence of macroinvertebrate assemblages in each zone down a river length. Following Rowntree et al. (2000), the channels of South African rivers may be classified into the following geozones, which are used MIRAI V2 and are also employed in the macroinvertebrate risk model (Table 4-6).

Table 4-5 Conceptualised relationship between taxon ecoregional confidence weighting and macroinvertebrate risk weighting.

Taxon ecoregional confidence weighting	Confidence description	Risk weighting
1	Low	Low risk (absence of taxon from observed sample indicative of low risk/impact to resource)
3	Moderate	Moderate risk (absence of taxon from observed sample indicative of moderate risk/impact to resource)
5	High	High risk (absence of taxon from observed sample indicative of potentially high risk/impact to resource)
A moderate risk is assumed when a taxon is present but was not expected		

Table 4-6 Geomorphological zonation of South African river channels (Rowntree et al., 2000).

Zone	Zone class	Gradient class
Zonation associated with a normal channel profile		
Source zone	S	Not specified
Mountain head water stream	A	>0.1
Mountain stream	B	0.04-0.099
Transitional	C	0.02-0.039
Upper Foothills	D	0.005-0.019
Lower Foothills	E	0.001-0.005
Lowland river	F	0.0001-0.0009
Zones associated with a rejuvenated profile		
Rejuvenated bedrock fall/cascades	Ar, Br or Cr	>0.02
Rejuvenated foothills	Dr or Er	0.001-0.019
Upland flood plan	Fr	<0.005

MIRAI V2 provides an estimation of the confidence weighting for macroinvertebrate taxa occurrence in a particular geozone. These confidence weighting are 1, 3 and 5, where 5 indicates the highest confidence weighting implying the highest assurance that the taxon does occur in the geozone, whereas 1 implies a very low confidence that the taxon does occur in the geozone, and 3 a moderate confidence weighting regarding the taxon occurrence within the geozone. Based on the geozone data, an impact on the macroinvertebrate assemblage is implied to have occurred: 1) if an expected taxon in the geozone was not observed; 2) if an unexpected taxon within the geozone was observed. The presence of an expected taxon in the observed data implies no impact or risk. The relationship between geozone confidence weighting and risk to the resource as conceptualised in the macroinvertebrate risk model is shown in Table 4-7.

The macroinvertebrate risk scores are generated by comparing the macroinvertebrates present at a site with those expected in that level 2 ecoregion and geozone under MIRAI V2. If those macroinvertebrates present are those that were anticipated, then no risk score is triggered. Likewise, if those macroinvertebrates not present at a site are those that were not predicted to be present in that level 2 ecoregion and geozone, no risk will be generated. In other words, risk is generated when something untoward happens, either by the absence of a taxon that should be there, or the appearance of a taxon that should not be present.

Table 4-7 Conceptualised relationship between taxon geozone confidence weighting and macroinvertebrate risk weighting.

Taxon geozone confidence	Confidence description	Risk weighting
1	Low	Low risk (absence of taxon from observed sample indicative of low risk/impact to resource).
3	Moderate	Moderate risk (absence of taxon from observed sample indicative of moderate risk/impact to resource).
5	High	High risk (absence of taxon from observed sample indicative of potentially high risk/impact to resource).
A moderate risk is assumed when a taxon is present but was not expected		

So, where presence and absence are scored as binary data, and where presence scores 1, the presence or absence of risk is predicted from observed and expected data (for that level 2 ecoregion/geozone) as shown below:

$$Risk\ presence = \ Observed\ XOR\ Expected$$

The above equation indicates whether risk is present or absent as a binary logical variable, with a value of 1 or TRUE indicating the presence of risk, and 0 or FALSE indicating the absence of risk as indicated by macroinvertebrate response.

This approach was suitable where a taxon was predicted to be present, but was in fact absent. This is because data were available indicating how good an indicator of ecoregion and geomorphological zone a given taxon may be. However, the reverse was not true. As a result of this, where a taxon was not predicted to occur, but was in fact present, a median risk score was assigned for ecoregion and geomorphological zone. Sensitivity scores were available, and were used to calculate risk in the same way.

Macroinvertebrates are known to be capable of a graded response to water quality stress (Odume et al., 2012). In the South African Scoring System version 5, macroinvertebrates are graded from score 1-15 according to their perceived sensitivity or tolerance to water quality stress (Dickens and Graham, 2002). Macroinvertebrates perceived to be very tolerant of water quality stress are awarded low scores, and those perceived to be highly sensitive, high scores, thus the scores 1-15 are in increasing order of perceived sensitivity to water quality stress. Using the SASS5 sensitivity scores, in MIRAI V2 macroinvertebrate taxa are graded into four sensitivity/tolerance categories as shown in Table 4-8. The relationship between macroinvertebrate sensitivity and risk/impact to the resource is conceptualised as an inverse one in the macroinvertebrate risk model (Table 4-8). The rationale is that highly sensitive macroinvertebrate taxa are usually the first to be affected even at low impact/risk to the resource. Only at higher risk/impact on the resource would the tolerant taxa be affected. That is losing a sensitive taxon might occur relatively easily, removing an insensitive taxon indicated some significant potential risk.

Therefore, when risk was indicated by a disagreement between what was observed and what was expected, the risk per taxon was calculated as follows:

$$Pooled\ risk = \sum Ecoregion\ presence, geozone\ presence, inverse(WQ\ sensivity\ score)$$

Pooled risk scores per taxon calculated in this way were then rescaled to give a range of 0-1. Finally, an overall score per sample was calculated by generating a mean of all the taxon scores to arrive at a sample ecoregion level 2 macroinvertebrate-based ecological risk estimation (Table 4-9).

Table 4-8 Conceptualised relationship between macroinvertebrate water quality sensitivity and risk/impact to the resource.

Sensitivity to water quality (WQ)	WQ sensitivity score	Risk weighting
Very low	1-3	Very high (a loss of taxon indicates potentially very high water quality impact/risk to the resource).
Low	4-7	High (a loss of taxon indicates potentially high water quality impact/risk to the resource).
Moderate	8-11	Moderate (a loss of taxon indicates potentially moderate water quality impact/risk to the resource).
High	12-15	Low (a loss of taxon indicates potentially very low water quality impact/risk to the resource).

4.3.1 Macroinvertebrate-based guidelines

An estimate of the amount of risk associated with changes in the macroinvertebrate community in any particular ecoregion level 2 and geozone location can be generated using the macroinvertebrate risk model outlined above. If the macroinvertebrate reference community perfectly matches the site or sample macroinvertebrate community, the site risk score would be zero, and it would be classified as an A category. As the community accumulates differences from the reference community, either through omission of taxa or insertion of new taxa, the risk score would accumulate. The boundary levels outlining the different categories is presented below in Table 4-9.

Table 4-9 Guideline derivation for Ecoregion level 2 and geozone macroinvertebrate risk estimates, corresponding to generic ecological categories of Kleynhans and Louw (2007).

Ecological category	Name	Upper boundary for rescaled risk	Description
A	Unmodified, natural	0.05	Unmodified and natural, expected and observed taxa are the same or extremely similar. Risk is very low.
B	Largely natural	0.2	A small change between the expected and observed taxa have taken place. Risk is low.
C	Moderately impacted	0.4	Moderate change has taken place between expected and observed taxa. Risk is moderate.
D	Largely impacted	0.6	Large change has taken place between expected and observed taxa. Risk is high
E	Seriously impacted	0.8	Serious change has taken place between expected and observed taxa, resulting in the loss of many taxa. The risk is very high and unacceptable.
F	Critically impacted	1	The macroinvertebrate assemblage has been critically modified, many taxa have been lost; the risk is extreme and unacceptable.

CHAPTER 5: SOUTH AFRICAN WATER QUALITITY GUIDELINES FOR FRESHWATER ECOSYSTEM: VERSION 2 – TIER 3

5.1 INTRODUCTION

Tier 3 assessment is triggered when risk is suspected based on the results of Tiers 1 and 2. Tier 3 provides a means for a site-specific water quality risk assessment by collecting detailed site-specific information. A key feature of Tier 3 assessments is that they are event/scenario-based. The reasoning behind this approach is that improving water quality implies a focus on the event/scenario driving water quality change rather than on the symptoms, which may manifest through a set of physico-chemical indicators or stressors such as reduced dissolved oxygen, excess nutrient and high levels of salts. By identifying the key event(s) responsible for observed changes, actions are thus better directed. The guidelines at Tier 3 are based on site-specific risk assessment and should be performed only by experts or a trained practitioner in ecological risk assessment. For the purpose of Tier 3 assessment, risk is conceptualized as a measure of the likelihood (probability) of an event/scenario/issue occurring and its adverse effects or consequence. This expression of risk is shown mathematically as:

Risk = (A, C, P), where **A** is the event or scenario, **C** is the consequence when A does occur, and **P** is the probabilities associated with **A** and **C**.

In the field of ecology, risk has received considerable attention, with the subdiscipline of ecological risk assessment (ERA) devoted to assessing and evaluating risk, and making risk-informed decision regarding ecosystem use and protection (Suter, 2006).The commonly applied definition of ERA is that put forward by the US Environmental Protection Agency (USEPA), which defined ERA as a “process that evaluates the likelihood that adverse ecological effects may occur or are occurring to ecosystems exposed to one or more stressors” (USEPA 1992, 1998; Chen et al., 2013). Claassen et al. (2001) suggested the adoption of this definition for South Africa. What is evident is that the conceptualisation of risk within ERA follows the conception of risk as the product of the likelihood of an event occurring and its consequence. Thus, risk within the context of ERA can be said to have the following dimensions:

- Event: the activity, agent, scenario, issues, or compound that initiate/trigger the risk, e.g. sedimentation, eutrophication or a development activity near a water resource.

- Receptor: the object, target, biological entity/agent upon which the event is likely to have an effect. In the case of the Tier 3 assessment, this would normally be the receiving/impacted water resource.

- Effect – the consequence, or outcome resulting from the interaction of the event and the receptor. The effect can be characterised in terms of its severity, type, magnitude, duration, or other similar measures.

- Probabilities: the likelihood of the stressor occurring and acting on the stressor, and the expression of the effect on the receptor. The probabilities can be characterised in terms of frequency of occurrence, frequency of impact and detection.

- Uncertainty: there is usually some level of uncertainty associated with the risk assessment, which may arise from the data, the risk assessment process or insufficient knowledge on some or all dimensions of the risk process. Uncertainty could be stochastic or epistemic uncertainty.

5.2 SITE-SPECIFIC WATER QUALITY RISK ASSESSMENT MODEL

A site-specific water quality risk assessment model was developed largely following DWS (2023) publication and drawing on the risk literature (e.g. Aven and Renn, 2009; Aven and Vinnem, 2007; Aven, 2010; Aven and Thekdi, 2018). The risk assessment model has three sub-models: 1) the consequence sub-model, 2) the likelihood sub-model and 3) the uncertainty sub-model.

5.2.1 Consequence sub-model

In the consequence sub-model, consequence is conceptualized as the sum of severity, duration and spatial scale (magnitude). Severity is determined as the effect on the water physico-chemistry and macroinvertebrate response. The physico-chemical severity is extrapolated from the percent Time Equal or Exceeded curve relative to the water quality guideline value for a predetermined ecological category A-F (read from either Tier 1 or Tier 2 Guidelines). Based on the percent Time Equal or Exceeded curve, the water physico-chemical severity is rated according to Table 5-1 Physical chemical severity rating based on the Percent Time Equal or Exceeded rating. The sub-model uses the average of the ratings for all physio-chemical variable to determine the overall severity rating for physico-chemistry.

Consequence *= sum (Severity, duration, spatial scale)*

Table 5-1 Physical chemical severity rating based on the Percent Time Equal or Exceeded rating

% Time equal or exceeded	Severity rating	Description
1-20	1	Very small and marginally harmful
21-40	2	Small and potentially harmful
31-60	3	Significant and slightly harmful, may be acceptable depending on the PES, EIS or REC
61-80	4	Great and very harmful; potentially unacceptable
81-100	5	Extremely harmful, disastrous and unacceptable

Macroinvertebrate response data are used in the sub-model to determine the biological dimension of the severity. The deviation of the observed data from the expected calculated based on the macroinvertebrate risk model (Tier 2) provides the basis for the rating of macroinvertebrate severity (Table 5-2). Where the macroinvertebrate risk model returns a deviation, corresponding to ecological category F, then the severity rating of 5 is awarded, whereas a deviation between the expected and observed assemblage corresponding to an ecological category B, corresponds to a severity rating of 1. An ecological category A has no severity rating, implying that the expected and observed assemblages are either the same or extremely similar.

Table 5-2 Macroinvertebrates severity rating as a function of the extent of deviation between the expected and observed taxa returned by the macroinvertebrate risk model in Tier 2.

Ecological category	Title	Upper boundary for rescaled risk	Description	Severity rating
A	Unmodified, natural	0.05	Unmodified and natural, expected and observed taxa are perfectly the same.	No rating
B	Largely natural	0.2	A small change between the expected and observed taxa have taken place. Risk is low.	1
C	Moderately impacted	0.4	Moderate change has taken place between expected and observed taxa. Risk is moderate.	2
D	Largely impacted	0.6	Large change has taken place between expected and observed taxa. Risk is high.	3
E	Seriously impacted	0.8	Serious change has taken place between expected and observed taxa, resulting in the loss of many biotas. The risk is very high and unacceptable.	4
F	Critically impacted	1	The macroinvertebrate assemblage has been critically modified, many biota have been lost; the risk is extreme and unacceptable.	5

The overall severity in the consequence sub-model is calculated as the average of the physico-chemical severity rating and that for the macroinvertebrate response.

The second dimension of the consequence sub-model is the duration. Exposure duration is an important aspect of risk assessment. The duration relates to the temporality of the event/scenario or compound that trigger the risk. The duration is rated as per Table 5-3. Event that occurs within a short period say one day to one month with no discernible impact on the water quality are rated lower compared to those occurring over a prolong period say one year with noticeable impact on the water quality status.

The third dimension of the consequence sub-model is the spatial scale, which quantify the spatial magnitude of the risk-triggering event. The spatial scale is rated in the consequence sub-model as per Table 5-4. Event that occurs within a confined/localized area are rated lower compared to those occurring over and affecting several catchments or resource units.

Table 5-3 Rating for the duration aspect of the consequence sub-model.

Duration of event/scenario	Rating	Description
One day to one month	1	An event occurring over a very short period, and has no noticeable effect on the water quality status.
One month to one year	2	An event occurring over a short period, the water quality status may be impacted but the status remains the same. The impact is not enough to change the water quality status.
One year to 5 years	3	An event occurring over a relatively long period, the water quality status may be impacted, there is a degradation of the water quality status. Mitigation/management action may improve the status.
5 years to 20 years	4	A long event in which the water quality status may be permanently degraded, and improvement is almost impossible.
More than 20 years	5	A very long event resulting in an extremely impacted water quality status, resulting in an F category, and no management action may result in any noticeable improvement.

Table 5-4 Rating for the spatial scale dimension of the consequence sub-model.

Duration of event/scenario	Severity rating	Description
Very localized	1	A confined and highly localized event.
Entire site	2	An event affecting an entire site.
Quaternary catchment	3	An event affecting and entire sites, extending down streams and affecting downstream resource, potentially more than one resource units.
Secondary catchment	4	A large event affecting an entire secondary catchment. Resources within the secondary catchment are affected. May affect multiple provinces.
Primary catchment and beyond	5	An event with large spatial scale, affecting the entire country and potentially beyond.

5.2.2 Likelihood sub-model:

The likelihood sub-model calculates the probability of the event occurrence, its impact and its detection. In the sub-model, likelihood is calculated as the sum of the frequency of occurrence of the risk-triggering event, frequency of the impact of the event and its detection, following DWS (2023).

***Likelihood** = Sum (Frequency of occurrence of the risk triggering event, frequency of impact, detection)*

The frequency of the risk triggering event refers to how often the event occurs. Events that occur rarely are rated lower compared to those that occur frequently or daily as shown in Table 5-5.

The frequency of impact relates to how often the occurrence of the event impact on the receiving water resource. This aspect is critical as the mere occurrence of an event does not necessarily translate to an impact. The frequency of impact is rated in the likelihood sub-model as shown in Table 5-6.

Table 5-5 Rating for frequency of occurrence of the risk-triggering event.

Frequency of occurrence	Rating	Description
Annually or more	1	An event that rarely occurs, mainly annually or more
Biannual	2	An event that occurs occasionally, mainly six monthly or more, but less than annually.
Monthly	3	An event that occurs monthly but less than six monthly.
Weekly	4	An event that occurs frequently, mainly weekly.
Daily or less	5	A highly frequent event, occurring daily or even hourly, creating a condition of persistence.

Table 5-6 Rating for frequency of impact of the risk-triggering event.

Frequency of impact (how often does the event impact on the receiving water resource?)	Rating	Description
>20%	1	An event/concern/scenario whose frequency of impact on the water quality is negligible.
>40%	2	An event that very seldom impacts the water quality or it is highly unlikely that it impacts on the water quality.
>60%	3	An event that occasionally impacts on the water quality
>80%	4	An event that often/regularly impacts on the water quality
>100%	5	An event that definitely impacts on the water quality

The early detection of a water quality risk-triggering event is critical for water resource protection. Events that are detected early enough may trigger the necessary management action or mitigation measures unlike those that are difficult to detect yet may have serious impact on water quality. The detection aspect of the likelihood-sub model allows for the rating of the ease with which the event or its impact may be detected as shown in Table 5-7.

Table 5-7 Rating for the detection of the risk-triggering event or its impact on the water quality component of the resource.

Detection	Rating	Description
Immediately	1	The effect on the water quality is immediate and can be detected easily
Without much effort	2	The effect on water quality may not be immediate but can be detected easily.
Require some effort to detect	3	The effect on water quality may not be easily observable and some effort is required to detect it.
Difficult to detect	4	The effect on water quality is difficult to observe and detect
Unnoticed	5	The effect on water quality may go unnoticed and is very difficult to detect.

5.2.3 Risk rating

The site-specific water quality risk assessment model returns an overall risk rating for a site by integrating the consequence and likelihood sub-models as per Table 5-8.

Table 5-8 Overall site-specific risk rating based on the consequence and likelihood sub-models.

Rating	Risk category	Description
1-20	Very low	Risk is acceptable.
21-40	Low	Risk is acceptable, water quality impact is minimal and easily managed/mitigated.
41-120	Moderate	Water quality risk are notable and require mitigation measures.
121-180	High	Water quality risk are very notable, may be long term and may require specialist mitigation measures.
181-225	Very High	Water quality risk is unacceptable and mitigation measures must be implemented to lower the risk.

5.3 UNCERTAINTY SUB-MODEL

The frequentist probability relates to relative frequency (Pf) (the relative fraction of time) the event occurs over a given period. In terms of water quality stressors for example, this can be said to be percent Time Exceeding or Equal the guideline value. The frequentist conception of probability construed uncertainty as the difference between the "estimated risk" and the true risk (Chapter 2). Mathematically the true probability of the concentration occurring at a level that may induced an adverse effect on the receptor can be expressed as Pf (A) and its estimate as Pf (A)*. Aven (2010) argues that this kind of uncertainty is better referred to as a variation rather than an uncertainty because it is not an uncertainty for the risk assessor/analyst. Following the frequentist approach, risk description can be represented as follows (Aven, 2010):

Risk description = (A, C,Pf*, P(Pf), K)

where K is the background knowledge that the estimate Pf* and the probability distribution P is based on.

The second interpretation of probability as earlier mentioned in Chapter 2 is that based on the Bayesian perspective (epistemic uncertainty). Uncertainty is subjective and is based on the assessor's background knowledge of the event/stressor and receptor. In the context of the site-specific water quality risk assessment for Tier 3, epistemic uncertainty is a critical element because of the complex interactions between aquatic ecosystems, their components, and the multitude of stressors.

Aven (2010) questioned the use of probabilities for expressing uncertainties, arguing that probabilities are inadequate. For this reason, several definitions of risk that expressly include uncertainties have been put forward in the literature. For example, Aven and Renn (2009) defined risk as an uncertainty of an event occurring, and its consequences. In the same vein, Rosa (1998, 2003) regard risk as when the outcome is uncertain where something of human value is at stake. A similar definition that expressly refer to uncertainty was also put forward by Jansen et al. (2019) as a combination of event occurring, its consequences and their associated uncertainties. Mathematically, the definition of risk in which uncertainties are made explicit can be expressed as:

Risk= (A,C,U)

where A is the object/event/stressor initiating the risk, C is the consequence and U, the uncertainty associated with A and C, and their underlying factors.

Based on this definition of risk, a risk description can be expressed as follows (Aven, 2010):

Risk description = (A, C, U, P, K)

where P is a subjective probability expressing U based on the background knowledge (K) of the assessor.

What is clear from this definition is an attempt to deal with uncertainty dimension inherent in risk assessment and evaluation. Fundamentally, these definitions are attempt to make uncertainty an explicit part of risk assessment, and this is key especially when dealing with complex systems such as freshwater ecosystems and a multitude of chemical and other stressors. For these reasons, at Tier 3 site-specific water quality risk assessment, attention is paid to the treatment of uncertainty, particularly epistemic uncertainty, which reflects the knowledge-based or judgemental dimensions of risk.

There are two important dimensions of epistemic uncertainty: (i) the knowledge upon which the probability is based, and (ii) the strength of the knowledge (Aven, 2017). Several factors may impact on the strength of the knowledge, and therefore the uncertainty associated with the water quality risk assessment and the decision made based on the outcome of the risk assessment.

The factors that needs to be considered include (Aven, 2017):

(i) The reliability and reasonability of the assumption made about the various metrics or components of the risk.

(ii) The adequacy of relevant, reliable data and information upon which the risk judgement is based.

(iii) The degree of agreement among experts and /or literature support for the various components of the risk being described or judged.

(iv) The degree to which the phenomenon in question is well-understood and whether it can accurately be modelled.

(v) A reflection on the extent of review of the knowledge upon which the risk judgement is based, particularly in relation to the so-called unknown known. The unknown known refers to a situation in which a particular knowledge may be available to other experts, but not to the risk assessor.

The reliability and reasonability of the assumptions made regarding the risk initiating event (e.g. a chemical pollutant or a development project), the receptor (e.g. ecosystem or its component), the consequence (e.g. the severity, duration, and magnitude of the effect), can be tested against expert judgements and/or empirical evidence. The estimation of uncertainty regarding reliability and reasonability of the assumption regarding the risk-triggering event is conducted for Tier 3 assessment following the scoring system in Table 5-9.

The adequacy of relevant, reliable data and information upon which risk judgement is based is a critical uncertainty consideration when conducting a site-specific water quality risk assessment. Since the confidence and reliability of the risk description and output rely heavily on data and information utilised, it is important that this aspect is fully and thoroughly considered. The uncertainties relating to the adequacy of relevant, and reliable data regarding physico-chemical and macroinvertebrate severities for Tier 3 assessment are scored as shown in Table 5-10 and Table 5-11.

Table 5-9 Uncertainty scoring regarding the reliability and reasonability of the assumption of the risk-triggering event(s).

Description of the risk triggering event	Score	Description of uncertainty
The risk is definitely attributable to the risk-triggering event.	1	Very low uncertainty/ very high confidence
The risk is largely attributable to the risk-triggering event. Although other events may contribute to the risk, such contribution(s) is/are largely negligible.	2	Low uncertainty/ high confidence
The risk is largely attributable to the risk-triggering event. Although the risk-triggering event may exist with other events, they may only moderately contribute to the risk being assessed.	3	Moderate uncertainty /moderate confidence
The risk triggering event occurs with other events/scenarios. The contribution(s) of other events/scenarios to the risk being assessed may be significant.	4	High uncertainty/ low confidence
The risk triggering event(s) occurs with other events/scenarios. It is impossible to attribute the risk only to the event(s) being assessed.	5	Very high uncertainty/ very low confidence

Table 5-10 Uncertainty scoring associated with the physico-chemical severity dimension of site-specific risk assessment.

Physico-chemical severity	Score	Description of uncertainty
Appropriate and relevant physico-chemical variables are selected, a minimum of 20 samples per selected variables are analysed. The sampling covers all seasons and more than 2 hydrological cycles. The data collector(s) is/are highly competent. There is a very high confidence in the data.	1	Very low uncertainty/ very high confidence
Appropriate and relevant physico-chemical variables are selected, a minimum of 15 samples per selected variables are analysed. The sampling covers all seasons and more than 2 hydrological cycles. The data collector(s) has/have received adequate training. There is a high confidence in the data.	2	Low uncertainty/ high confidence
Appropriate and relevant physico-chemical variables are selected, a minimum of 10 samples per selected variables are analysed. The sampling covers all seasons and at least a hydrological cycle. The data collector(s) has/have received some training. The confidence in the data is moderate.	3	Moderate uncertainty /moderate confidence
Some relevant physico-chemical variables are selected, a minimum of 5 samples per selected variables are analysed. The sampling covers some seasons. The data collector(s) received some training. Confidence in the data is low.	4	High uncertainty/ low confidence
Some relevant physico-chemical variables are selected, a minimum of one sample per selected variables are analysed. The sampling cover at least a season. The data collector(s) received some training. Confidence in the data is very low.	5	Very high uncertainty/ very low confidence

Table 5-11 Uncertainty scoring associated with the macroinvertebrate severity dimension of site-specific risk assessment.

Macroinvertebrate severity	Scoring	Description of uncertainty
A minimum of eight samples were collected, covering all seasons. The data collector is SASS-5 accredited.	1	Very low uncertainty/ very high confidence
A minimum of six samples were collected, covering all seasons. The data collector is SASS-5 accredited.	2	Low uncertainty/high confidence
A minimum of four samples were collected, may or may not have covered all seasons. The data collector is SASS-5 accredited or may have received some training.	3	Moderate uncertainty/moderate confidence
A minimum of 2 samples were collected. The data collector is SASS5 accredited or may have received some training.	4	High uncertainty/low confidence
A minimum of one sample collected. The data collector is SASS5 accredited or may have received some training.	5	Very high uncertainty/very low confidence

Agreement among experts can provide a measure of the strength of knowledge upon which the risk judgement is based. Generally, when there is a broad agreement among experts about the risk judgement, then the knowledge upon which the risk judgement is made can be consider as generally strong. On the other hand, strong disagreement among experts suggests weak knowledge and potentially high level of uncertainty. Assessing the level of agreement among experts is thus an integral part of the uncertainty assessment sub-model for Tier 3 risk assessment (Table 5-12).

Table 5-12 Assessing the level of expert agreement/disagreement/literature support at Tier 3 site-specific risk assessment.

Expert agreement/ literature support	Score	Description of uncertainty
The agreement between experts or literature support for the rating of the likelihood metrics and the duration of the risk-triggering event is very high.	1	Very low uncertainty/ very high confidence
The agreement between experts or literature support for the rating of the likelihood metrics and the duration of the risk-triggering event is high.	2	Low uncertainty/ high confidence
There is some agreement between experts or literature support for the rating of the likelihood metrics and the duration of the risk-triggering.	3	Moderate uncertainty /moderate confidence
There is little agreement between experts or literature support for the rating of the likelihood metrics and the duration of the risk-triggering.	4	High uncertainty/ low confidence
There is serious disagreement between experts or very little literature support for the rating of the likelihood metrics and the duration of the risk-triggering.	5	Very high uncertainty/ very low confidence

The degree to which the phenomenon in question is well-understood and whether it can accurately be modelled is an important factor when considering the strength upon which the risk judgement is based. Here, a systematic analysis of the extent to which the source of the risk initiating event/stressor, the receptor, and its effects, are understood is critical. If the understanding of any of these dimensions influencing the risk judgement is poor, then the knowledge upon which the risk judgement is made can be considered low, leading to a potentially high level of uncertainty associated with the risk judgement. Similarly, a reflection on the extent of review of the knowledge upon which the risk judgement is based, particularly in relation to the so-called unknown known, is important. The unknown known is an important consideration for the Tier 3 assessment. The site-specific underlying factors which may impact on the risk may not always be known to the risk assessor yet may be common knowledge to other experts (Table 5-13).

Table 5-13 Uncertainty assessment regarding the risk assessor's knowledge of the site-specific risk modifying factors.

Knowledge of site-specific risk modifying factors	Score	Description of uncertainty
The knowledge of site-specific risk modifying factors is very high. Comprehensive data such as geology, soils, climate, vegetation, hydrology, social-economic context, etc. have been collected/ or are available and analysed.	1	Very low uncertainty/ very high confidence
The knowledge of site-specific risk modifying factors is high. Adequate data such as geology, soils, climate, vegetation, hydrology, social-economic context, etc. have been collected/ or are available and analysed.	2	Low uncertainty/ high confidence
The knowledge of site-specific risk modifying factors is moderate. Some data such as geology, soils, climate, vegetation, hydrology, social-economic context, etc. have been collected/ or are available and analysed.	3	Moderate uncertainty /moderate confidence
Little is known about the site-specific risk modifying factors. Very little data is available on the site regarding factors that may modify the risk.	4	High uncertainty/ low confidence
Nothing is known about the site-specific risk modifying factors. No data are available on the site regarding factors that may modify the risk.	5	Very high uncertainty/ very low confidence

5.3.1 Overall uncertainty/confidence rating

The overall rating for the uncertainty and confidence level associated with the site-specific water quality risk assessment model is interpreted as per Table 5.14.

Table 5-14 Overall uncertainty rating associated with the site-specific water quality risk assessment.

Rating	Confidence level	Description
1-5	Very high	The uncertainty associated with the risk assessment is acceptable.
6-10	High	The uncertainty associated with the risk assessment is minimal and acceptable.
11-15	Moderate	The uncertainty associated with the risk assessment is notable.
16-20	Low	The uncertainty associated with the risk assessment is high. Steps should be taken to reduce the uncertainty and improve the confidence level.
21-25	Very low	The uncertainty associated with the risk assessment is very high. Steps should be taken to reduce the uncertainty and improve the confidence level.

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