Environ Sci Pollut Res (2014) 21:118–130
DOI 10.1007/s11356-013-1780-0

ENVIRONMENTAL QUALITY BENCHMARKS FOR PROTECTING AQUATIC ECOSYSTEMS

Site-specific water quality guidelines: 1. Derivation approaches based on physicochemical, ecotoxicological and ecological data

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Received: 31 January 2013 / Accepted: 26 April 2013 / Published online: 12 July 2013

Abstract Generic water quality guidelines (WQGs) are developed by countries/regions as broad scale tools to assist with the protection of aquatic ecosystems from the impacts of toxicants. However, since generic WQGs cannot adequately account for the many environmental factors that may affect toxicity at a particular site, site-specific WQGs are often needed, especially for high environmental value ecosystems. The Australian and New Zealand Guidelines for Fresh and Marine Water Quality provide comprehensive guidance on methods for refining or deriving WQGs for site-specific purposes. This paper describes three such methods for deriving site-specific WQGs, namely: (1) using local reference water quality data, (2) using biological effects data from laboratory-based toxicity testing, and (3) using biological effects data from field surveys. Two case studies related to the assessment of impacts arising from mining operations in northern Australia are used to illustrate the application of these methods. Finally, the potential of several emerging methods designed to assess thresholds of ecological change from field data for deriving site-specific WQGs is discussed. Ideally, multiple lines of evidence approaches, integrating both laboratory and field data, are recommended for deriving site-specific WQGs.

Keywords Water quality guidelines · Site specific · Reference data · Toxicity · Field studies

Responsible editor: Philippe Garrigues

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Introduction

The contamination of aquatic ecosystems with natural and anthropogenic chemical substances (referred to herein as toxicants) has been identified as a key global threat to water security and biodiversity (Vorosmarty et al. 2010). As such, it is essential that we understand, as best as possible, the amounts (i.e. concentrations and/or loads) of toxicants that can exist in aquatic ecosystems without causing unacceptable environmental harm. Internationally, the key means for assessing the protection of aquatic ecosystems from toxicant impacts is through the derivation and application of water (and/or sediment) quality guidelines (WQGs; also variously termed benchmarks, triggers, limits, thresholds, standards and criteria; although important differences in terminology definitions do exist between jurisdictions). Water quality guidelines are science-based numerical concentrations that represent the level of risk that the community is willing to take based on what it believes the environment can withstand and the ecosystem condition it is prepared to accept (ANZECC/ARMCANZ 2000; Leung et al. 2013).

Water quality guidelines are typically derived at the national level (e.g. Australia and New Zealand–ANZECC/ARMCANZ

(2000); Canada–Canadian Council of Ministers of the Environment (2007); The USA–U.S. Environment Protection Agency (2012)) or, in the case of Europe, at a multi-national level (European Commission 2011). From a regulatory point of view, broad-scale generic WQGs represent the most efficient approach to water quality management across large spatial scales. However, generic WQGs cannot adequately account for (1) the myriad environmental (physicochemical and biological) conditions in aquatic ecosystems that can affect toxicant fate, bioavailability and, ultimately, toxicity and (2) differences in species' sensitivities across ecosystem types (Carlson et al. 1984; ANZECC/ARMCANZ 2000; Canadian Council of Ministers of the Environment 2003). Consequently the development of regional or even site-specific WQGs is often needed, particularly where the generic WQGs are likely to be too under-protective or over-protective (due to either or both physicochemical and biological factors), or carry too much uncertainty (e.g. where there may be locally important species or ecosystems that are not represented in the toxicity data set used to derive the generic WQGs). The derivation of site-specific WQGs is not a straightforward process and requires extensive knowledge of the toxicant(s) and ecosystem being assessed. In recognition of this, considerable guidance on the topic has been published (Carlson et al. 1984; ANZECC/ARMCANZ 2000; Canadian Council of Ministers of the Environment 2003).

Methods by which site-specific WQGs can be derived vary from simple modifications of the relevant generic WQG to completely new derivations based on site-specific physicochemical data and/or local biological effects data. Specific approaches vary amongst countries, but they generally comprise similar guiding principles (e.g. quality of site-specific data is paramount; confidence in the relevance and accuracy of the site-specific WQG must be greater than the generic WQG). Although comprehensive guidance has been available in some places for at least a decade (ANZECC/ARMCANZ 2000; Canadian Council of Ministers of the Environment 2003), as Leung et al. (2013) point out, methods for the derivation of site-specific WQGs require continual improvement to incorporate the most recent research findings.

In this paper, we describe the methods for site-specific WQG derivation recommended by the Australian and New Zealand Guidelines for Fresh and Marine Water Quality (ANZECC/ARMCANZ 2000), and use case studies to illustrate their application. At the time these guidelines were published, they represented the most comprehensive guidance for dealing with this issue. The purpose of this paper is to use examples from our experience to illustrate the multiple ways in which site-specific WQGs can be derived. We also cast an eye to the future and discuss some emerging approaches and statistical techniques that may further improve the derivation of site-specific WQGs.

Overview of ANZECC/ARMCANZ (2000) guidance for deriving WQGs

The water quality assessment framework promoted by ANZECC/ARMCANZ (2000) comprises a hierarchy of methods for deriving WQGs. Most preferred is the use of local biological effects data, which may be acquired from toxicity tests, including multiple species toxicity tests (i.e. laboratory or field micro/mesocosms) or field biological data. If such data are not available, the derivation of WQGs from local reference data applicable to the site being assessed (the test site) is the next preferred method. This referential approach applies mostly to physical and chemical stressors (*sensu* ANZECC/ARMCANZ (2000)) such as pH, turbidity and electrical conductivity (EC), and for toxicants in water and/or sediment where natural background concentrations exceed the generic national WQGs. If local reference data cannot be used because they do not meet certain acceptability requirements for quantity and quality, the generic WQGs (nationally based for toxicants, regionally based for physicochemical stressors) can be tailored to local environmental conditions to some degree using various decision frameworks. For toxicants, the decision tree includes consideration of factors such as natural background concentrations, analytical quantitation limits and various toxicity-modifying factors (e.g. water hardness, pH, dissolved organic carbon) that might warrant an adjustment to the generic WQG. Finally, the least preferred method is to use the generic, unadjusted WQGs as they are provided.

The environmental condition of, and associated level of protection for, a site can also inform the selection/derivation of WQGs to make them more site-specific. For example, a location with a high conservation/ecological value may need to be afforded higher levels of protection and, therefore, require more stringent WQGs, than the default condition would require. This may involve assigning a 99 % species protection WQG instead of the default 95 % species protection WQG value that would otherwise apply, or even requiring the derivation of a WQG using local biological effects data. Conversely, sites that are already highly disturbed may be assigned a lower level of protection and a less stringent WQG than the default, although this may need to be done within an overarching tenet of continual improvement and the need to consider cumulative impacts.

Under the ANZECC/ARMCANZ (2000) framework, WQGs are implemented through water quality objectives (WQOs). WQOs are typically represented by numerical concentrations or narrative statements that have been established to support and protect the designated uses of water at a specific site. They are based on the scientifically derived WQGs but may be modified by other inputs such as additional scientific information and social, cultural, economic or political constraints.

Thus, the ANZECC/ARMCANZ (2000) water quality assessment framework provides several ways in which WQGs (and WQOs) can be refined or derived for site-specific purposes. We have applied the framework in a number of situations, particularly in relation to the protection of aquatic ecosystems from (potential) impacts arising from mining activities. The current paper first describes, and then illustrates, three of the above-mentioned methods for deriving site-specific WQGs, namely: (1) using local reference data, (2) using biological effects data based on laboratory-based toxicity testing and (3) using biological effects data from field surveys.

ANZECC/ARMCANZ (2000) methods for deriving site-specific WQGs

Site-specific guidelines derived from local reference data

As noted above, the use of local reference data to derive site-specific WQGs is generally preferred over the use of generic (default) WQGs. For toxicants, this approach is recommended particularly when natural background concentrations are higher than the generic WQG. However, this method may also be preferred in areas of high conservation/ecological value if stakeholders are not prepared to accept less stringent generic guidelines that would otherwise apply (ANZECC/ARMCANZ 2000; Canadian Council of Ministers of the Environment 2003), even if these are generally accepted as providing full protection of receiving water environments.

To derive a site-specific WQG using reference site data, detailed water quality chemistry data should be available over at least a 2-year period from a reference site un-impacted by the relevant toxicant(s). If knowledge of the system suggests it is necessary (e.g. large seasonal difference in flow regime and/or water quality) and if the dataset is large enough, site-specific WQGs may also need to be derived for distinct seasonal (or other, e.g. diurnal) periods. The 80th percentile of the distribution of the natural background concentration is taken to represent the site-specific WQG. This is then compared to the median value from the test site dataset. This comparison is not biologically/ecologically based, rather it is to identify a measurable perturbation at the test site relative to the reference site. Whether or not an exceedance of a local reference-based WQG at the test site has biological and/or ecological ramifications cannot be determined without more comprehensive investigation (ANZECC/ARMCANZ 2000). The ANZECC/ARMCANZ (2000) framework differs slightly from some other reference data approaches, typically in relation to the selected “background” value from the reference data (e.g. 90th percentile, mean plus two standard deviations; Canadian Council of Ministers of the Environment 2003), but the general principles are the same.

Site-specific guidelines derived from laboratory based toxicity data

The ANZECC/ARMCANZ (2000) decision framework for assessing water quality associated with toxicants provides the option to undertake direct toxicity assessment at a number of decision points. This can be required: when a generic WQG does not exist or is only a ‘low reliability’ value (i.e. a WQG based on the lowest of only three toxicity values); when the generic WQG is exceeded; when there are locally important species that require specific toxicological data for protection; when the composition of local water is either substantially different to that usually observed and/or contains components that may significantly influence toxicant bioavailability and toxicity; and when there are mixtures of toxicants present.

The key aim of undertaking site-specific toxicity studies is to increase understanding of how a toxicant(s) may adversely affect biota under the relevant environmental conditions, such that more appropriate WQGs can be derived. ANZECC/ARMCANZ (2000) provides comprehensive guidance on the conduct of site-specific toxicity assessments. This guidance includes selection of appropriate local or regionally relevant test species, dilution water, biological endpoints and statistical estimates, other test design considerations (e.g. acute vs chronic, single chemical vs complex mixture, laboratory vs in situ), and Quality Assurance and Quality Control considerations.

Species sensitivity distributions (SSDs) are the preferred method for deriving site-specific WQGs using toxicity data, where the WQG is represented by a specific percentile, typically the 5th percentile (i.e. representing protection of at least 95 % of species) of a cumulative probability distribution of the relevant toxicity data for the toxicant. ANZECC/ARMCANZ (2000) guidance recommends using chronic toxicity test results for at least five species from a minimum of four taxonomic groups and deriving the WQG from a SSD. However, a current review of the guidance has recommended that data from at least eight species are used (Warne et al. 2013). As noted above, a different percentage of protected species can be selected, depending upon the agreed ecosystem condition and protection level. Similar guidance for the conduct of toxicity testing using local species and local waters for deriving site-specific WQGs is provided in other countries (Carlson et al. 1984; Canadian Council of Ministers of the Environment 2003). In contrast, the European Union recommends bioavailability-based models, such as biotic ligand models (European Commission 2011).

Notwithstanding the value of local species’ toxicity data, the degree of protectiveness of laboratory-based WQGs should be verified with field data. An integrated monitoring and assessment approach, where multiple lines of evidence are used to provide assurance of an appropriate level of ecosystem protection, is promoted by ANZECC/ARMCANZ (2000) and has also been recommended in the USA (Cormier et al. 2009). Field-based approaches are discussed in the following section.

Site-specific guidelines derived from field biological data

The use of biological effects information to derive site-specific WQGs extends to the use of data from field assessments. Whilst ANZECC/ARMCANZ (2000) is not prescriptive on how to derive WQGs from field data, the framework does provide extensive guidance on how to design appropriate field biological studies for identifying unacceptable levels of change. It advises that a WQG be defined as the concentration of toxicant(s) below which ecologically or biologically meaningful changes do not occur. Such WQGs can be refined more or less conservatively, and even agreed as WQOs (see previous discussion of WQOs), depending on factors such as the level of protection of the water body, and after consultation with stakeholders. In order to use field data to derive a site-specific WQG for a given toxicant there must be sufficient data to establish a biological response-water quality relationship, and confidence that the effects are caused by the specific toxicant. With respect to the latter, field observational data are often confounded by habitat, biological and other water quality issues unrelated to the toxicant in question.

Numerous methods have been used and promoted for detecting changes/thresholds in field-based metrics associated with water quality changes. In the case studies below, we provide examples that illustrate the use of multivariate analyses and field-based SSDs.

Case study 1: Ranger uranium mine

The Ranger uranium mine is located in the Alligator Rivers Region (ARR) of the Northern Territory of Australia, approximately 250 km east of Darwin, and is surrounded by the World Heritage and Ramsar-listed wetlands of Kakadu National Park. The climate is wet–dry tropical, with the majority of the average annual rainfall of 1,580 mm occurring between November and April each year. During much of this time, mine waters are discharged to a key regional waterbody, Magela Creek, which lies in close proximity to the mine site. To ensure the highly valued aquatic ecosystems of the Magela Creek catchment are protected from U mining, an integrated assessment and monitoring program has been in place since the mid-1980s. The overall program involves comprehensive chemical, ecotoxicological and biological monitoring and research, and has been described in detail elsewhere (Humphrey et al. 1999; van Dam et al. 2002; Jones et al. 2009). Some of the elements relevant to the derivation of site-specific WQGs are described below.

Reference site data

The reference data approach has been used to derive site-specific WQGs for pH, EC, turbidity, and trace metals and major ions of concern for which site-specific biological effects data are not available, for Magela Creek downstream of the Ranger mine (Iles 2004). In this case, the reference site is located in Magela Creek upstream of any inputs from the mine operations. The approach has been further enhanced by developing a water quality trigger framework that incorporates a hierarchy of reference data-based WQGs, exceedances of which trigger increasingly strict reporting and investigation requirements by the mine's operator (Iles 2004). The framework consists of Focus, Action and Guideline trigger levels that correspond to site-specific WQGs based on the 80th, 95th and 99.7th percentiles, respectively, of the reference site distributions. Given the high conservation/ecological value of the aquatic ecosystem, exceedance of a WQG in just a single measured sample (as opposed to the median of a dataset as normally required) at the test site downstream of the mine necessitates that the appropriate action be taken depending on which trigger level is exceeded.

The example provided here is for manganese (Mn). Although not naturally elevated above the ANZECC/ARMCANZ (2000) national WQG of 1,200 μg/L (99 % species protection; applicable to high conservation/ecological value ecosystems), the national WQG was considered inappropriate because it was over two orders of magnitude above the median natural background Mn concentration of 4.7 μg/L. Since the low pH (5.5–6.5) and hardness (<6 mg/L as $CaCO_3$) waters of Magela Creek favour Mn bioavailability (Peters et al. 2011), the national WQG may be under-protective in this situation. As site-specific biological effects data were not available, nor was their acquisition assigned a high priority at the time, the use of the reference site approach for Mn was considered most appropriate for this site.

Descriptive statistics for the reference site dataset, and the resultant site-specific Focus, Action and Guideline trigger levels, are shown in Fig. 1. Manganese represents a special case of the reference site approach, whereby specific knowledge of the interaction between hydrology and water chemistry of Magela Creek enabled the assessment of water quality against the WQG trigger levels to be tailored for the local situation, as described below. Concentrations of Mn in surface water in Magela Creek downstream of the mine are largely governed by two key processes: (1) expression of groundwater containing naturally higher concentrations of Mn, typically during the beginning and end of the wet season when creek flow is low and mine water is not being discharged; and (2) surface water influence during the main part of the wet season, when mine waters are usually being discharged. Analysis of the time series Mn data from the test site confirmed that higher Mn concentrations

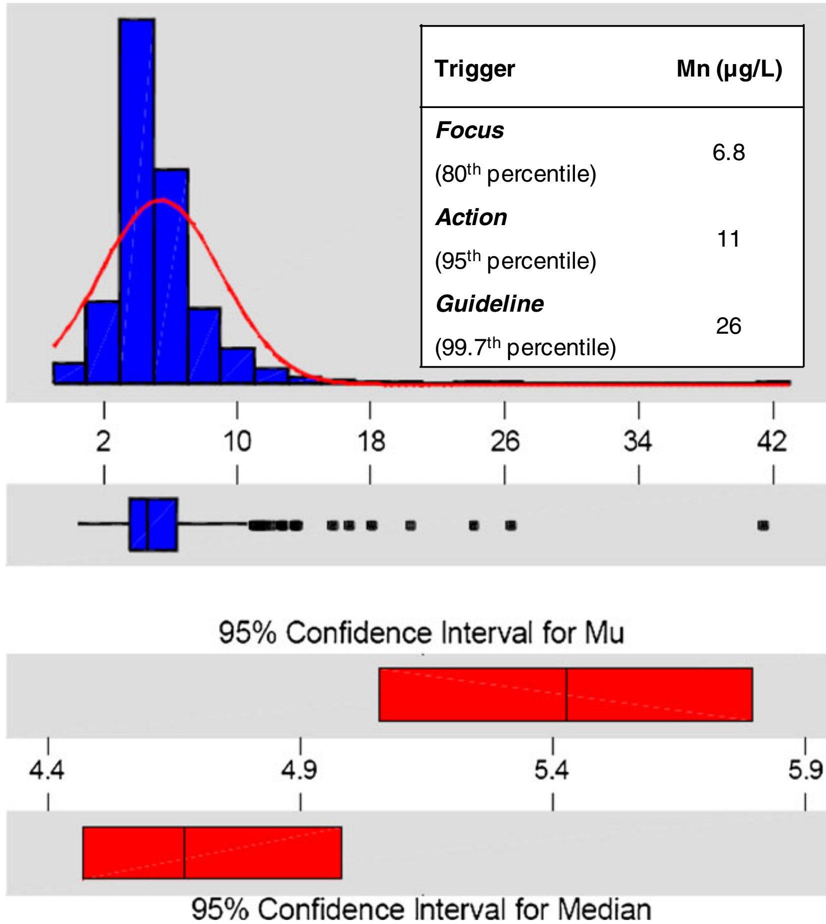

Fig. 1 Frequency distribution, *box plot* and mean (Mu) and median statistics for manganese (0.45 μm filtered) at the Magela Creek reference site (data from 1993 to 2003, n=365). After (Iles 2004). Focus, Action and Guideline values are shown in the *inset box* in the frequency distribution plot

occurred at creek flows of ≤5 m^3/s than at >5 m^3/s (Iles 2004) (Fig. 2). As these low creek flows and associated instances of elevated Mn occur outside the periods of mine water discharge, the site-specific WQG trigger levels for Mn are only applied at the test site when creek flow is >5 m^3/s. Figure 2 shows that when creek flow is >5 m^3/s, exceedance frequencies of the three WQG trigger levels are broadly as expected based on the percentiles of the reference data that

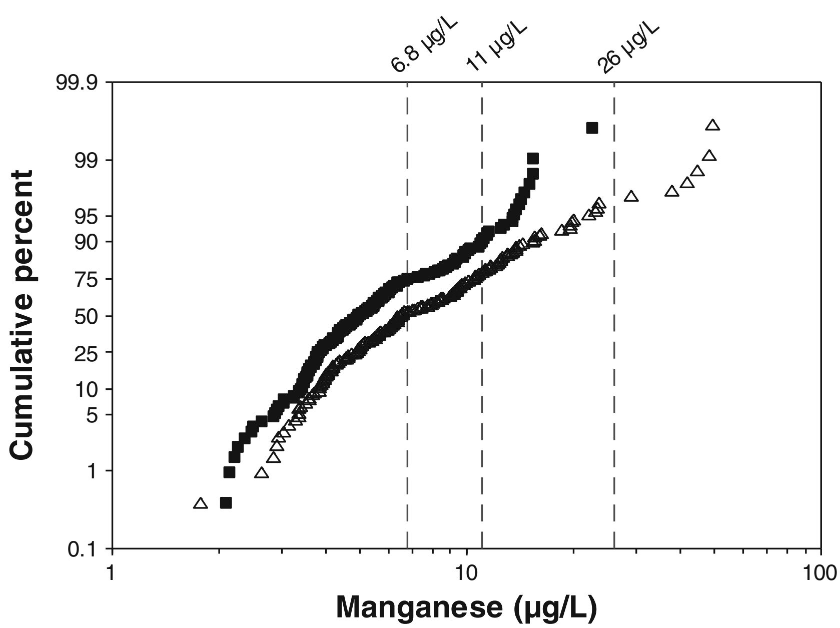

Fig. 2 Comparison of measured concentrations of manganese downstream of the mine since 2001 (*filled square*, flow >5 m3/s, n=182; *triangle*, flow ≤5 m3/s, n=188) with the reference-based Focus (6.8 μg/L), Action (11 μg/L) and Guideline (26 μg/L) trigger levels

the trigger levels represent (i.e. they reflect upstream water quality and there appears to be negligible mine influence). This example highlights the need to have a comprehensive understanding of a site in order to derive and apply site-specific WQGs in an appropriate assessment context. It is noteworthy that Mn toxicity testing using local species has recently been undertaken, and toxicity-based WQGs may ultimately replace the existing local reference data-based WQGs.

Local toxicity data

Site-specific toxicity data have been used to derive local WQGs for the two key toxicants associated with the Ranger mine, namely U and magnesium (Mg). The requirement for WQGs based on site-specific toxicity data was brought about by two scientific and two socioeconomic reasons. From a scientific perspective, (1) there was no existing national WQG for Mg, while there was only a low reliability national WQG of 0.5 μg/L for U and (2) the characteristic physicochemistry of Magela Creek waters (i.e. the low pH and hardness noted above, as well as low ionic strength [<20 μS/cm] and alkalinity [<10 mg/L as CaCO3]) would be likely to favour metal bioavailability and toxicity. From a socioeconomic perspective, (1) the high ecological value of the region's aquatic ecosystems necessitated data for local freshwater species; and (2) the need for mining to continue in the context of unavoidable low level inputs of U and Mg from the mine site into Magela Creek meant that that reference-based WQGs could not be used as effective management tools for these toxicants. Specific details of the derivation of the site-specific WQGs for both U and Mg are provided below.

For both U and Mg, SSDs based on local species toxicity data were used to derive the site-specific WQGs. Whilst promoting the use of local species toxicity data for deriving site-specific WQGs, ANZECC/ARMCANZ (2000) cautions against excluding comprehensive datasets for non-local species in favour of potentially small datasets for local species, whereby the resulting WQG may be no more, or even less, robust. In the case of U and Mg, however, there was no choice but to use only local species data, as very few data already existed in the literature and, where they did exist, they were not applicable to the unique physicochemical conditions of Magela Creek water.

For both metals, toxicity was assessed in Magela Creek water for at least five freshwater species local to Magela Creek, using metal salts (uranyl sulfate and magnesium sulfate) containing the most appropriate companion anion (sulfate) present in the Ranger mine waters. The test environmental conditions were consistent with the regional tropical climate (i.e. 27 °C, 12-h/12-h photoperiod). Due to the high ecological value of the region's aquatic ecosystems, the 1st percentile from the local species' SSDs, equating to protection of at least 99 % of species, was taken as the site-specific WQG.

A site-specific WQG for U was derived in the mid-2000s, once chronic U toxicity data for five local species (a microalga, macrophyte, microcrustacean, cnidarian and fish) were available and published (Hogan et al. 2005). The SSD based on no-observed-effect concentrations for the local species is shown in Fig. 3. The 99 % species protection WQG derived from the SSD of 6 μg/L is currently used as a regulatory "Limit". Limits represent an additional category of trigger value within the water quality trigger framework for the ARR. As they are based on local species' toxicity data, Limits are the most stringent of the trigger values and, as such, represent concentrations that are not to be exceeded in Magela Creek. In addition, the lower 95 % and 80 % confidence limits of the U Limit, of 0.3 and 0.9 μg/L, respectively, are assigned as Focus and Action trigger levels, respectively (Iles 2004), which are consistent with the water quality management approach described in the previous section. Thus, this approach to setting the lower trigger levels takes into account the uncertainty in the ecotoxicologically-based Limit value for U.

Figure 3 also compares the site-specific WQG and its associated trigger levels to the distribution of U concentrations measured in Magela Creek downstream of the mine since 2001. This comparison shows that the Limit and Action levels have not been approached, while the Focus level has been exceeded on less than 0.5 % of sampled occasions (measured as weekly grab samples during the periods of creek flow). This indicates that the appropriate settings are in place to manage mine water discharges whilst ensuring that the environment remains protected.

Since the site-specific WQG for U was implemented, further U toxicity data for local species have been published (Cheng et al. 2010; Hogan et al. 2010; van Dam et al. 2012). In addition, the influence of natural dissolved organic carbon (DOC), which is a key modifier of U toxicity, has been quantified for several local species (Trenfield et al. 2011). These data have been used to develop a DOC correction algorithm that increases the U WQG by approximately 10 % for every 1 mg/L increase in DOC concentration (van Dam et al. 2012). These recent enhancements to the site-specific U toxicity dataset are currently being incorporated into a revision of the site-specific U WQG.

Although U is a toxicant of high public concern, Mg poses the greatest potential risk to aquatic biota, based on measured time series concentration data. Results of aquatic macroinvertebrate surveys conducted in the mid-1990s found a strong correlation between EC and changes in community assemblages of billabongs (lentic waterbodies) along a gradient of mine water exposure (O'Connor et al. 1997). As EC in Ranger mine waters is dominated by

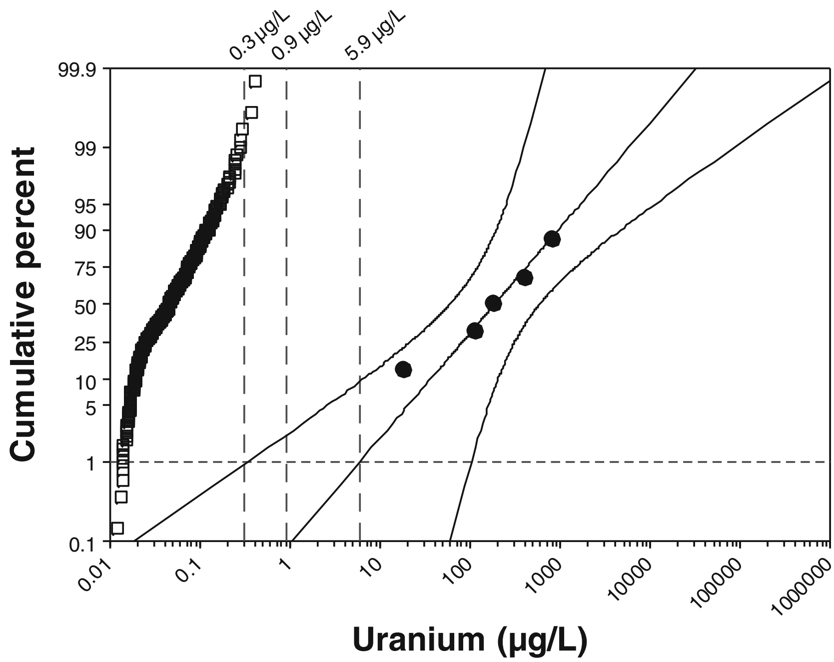

Fig. 3 Species sensitivity distribution of chronic uranium toxicity data (*filled circle*, n=5, as no-observed-effect concentrations) for species local to Magela Creek, based on data reported by Hogan et al. (2005). The data are fitted with a log-logistic distribution with associated 95 % confidence limits shown. Also plotted are the measured concentrations of uranium downstream of the mine since 2001 (*square*, n=469). The *horizontal reference line* represents the 1st percentile, while the *vertical reference lines* show the 99 % species protection value (5.9 µg/L) and the lower 80 % confidence limit (0.9 µg/L) and lower 95 % confidence limit (0.3 µg/L) of this value

$MgSO_4$, a study was initiated to generate site-specific toxicity data and derive a site-specific WQG. The initial study (van Dam et al. 2010) assessed the toxicity of $MgSO_4$ to six local freshwater species (a microalga, macrophyte, microcrustacean, cnidarian, gastropod and fish). The study found that Mg was the dominant toxic ion (and, hence, much of the subsequent research focused on Mg rather than SO_4), and also that Mg toxicity was reduced with increasing Ca concentration. Using the SSD approach, a site-specific 99 % species protection WQG of 2.5 mg/L (rounded to 3 mg/L for operational purposes; see Sinclair et al. (2013)) was derived for a Mg/Ca (mass) ratio of ≤9:1 (van Dam et al. 2010). As this study was being completed, the implementation of continuous EC monitoring in Magela Creek downstream of the mine showed that mine water discharges were typically being manifest as short duration (i.e. minutes to hours) pulses, sometimes in excess of the site-specific Mg WQG. The driver for the shorter duration pulses is a complex interplay between water level in Magela Creek and the flow lines discharging surface water from the mine site.

Consequently, a new study was initiated (Hogan et al. 2013), whereby the toxicity of $Mg(SO_4)$ pulse exposures in Magela Creek water to six local freshwater species (as tested above) was assessed. Using the SSD approach, the study derived site-specific 99 % species protection WQGs for 4-h, 8-h and 24-h Mg pulse exposures of 94 mg/L (1,140 µS/cm), 14 mg/L (174 µS/cm) and 8.0 mg/L (102 µS/cm), respectively. In conjunction with the continuous exposure WQG of 3 mg/L (42 µS/cm), the data were used to generate a site-specific WQG versus exposure duration model, from which duration-specific Mg/EC WQGs can be derived. Thus, this site-specific derivation of a WQG has not only captured the local species and local water elements, but also the actual nature of the toxicant exposures. The toxicity and model development aspects of the study are detailed by Hogan et al. (2013), while the subsequent proposed implementation of the model into the regulatory framework, including an assessment against environmental concentrations, is detailed by Sinclair et al. (2013).

The two examples provided here illustrate the approach to deriving site-specific WQGs using toxicity data from local species in local waters. However, site-specific toxicity assessments require substantial time to complete and are expensive to conduct. Hence, the potential benefits of this approach must be able to be demonstrated, and the testing program must be carefully planned and appropriately executed. In the case of the above examples, the local species toxicity test methods were already established as part of a 20+ year program of research and monitoring on the impacts of U mining in the ARR.

Local field biological data

Field-based biological effects data have not been able to be used to derive site-specific WQGs for Magela Creek downstream of the Ranger mine because water quality at the compliance site has never deteriorated to the point at which field effects have been detected by the long-term multiple lines of evidence chemical and biological monitoring program that is in place (Supervising Scientist 2012). Whilst the monitoring results clearly show that the existing WQGs derived using a combination of local reference data and site-specific laboratory toxicity methods (described above) provide adequate environmental protection in the receiving waters of Magela Creek, the actual threshold for field effects is unknown.

However, field biological data are being used to derive site-specific WQGs for mine water-contaminated billabongs located immediately adjacent to the mine site (as opposed to the downstream compliance point within Magela Creek). The billabongs lie along the catchment flow lines for discharge of surface runoff from the mine site and discharge into Magela Creek. The EC in these billabongs is elevated above natural background levels. A site-specific WQG for EC for the billabongs is being derived based on those periods of the water quality (EC) record that support an ecological condition (based primarily on macroinvertebrate community data) no different to that found in regional reference billabongs. The details of this work have been described elsewhere (Humphrey et al. 2012). The outputs from a number of multivariate analysis methods, including multi-dimensional scaling and Analysis of Similarity (Clarke 1993), the latter quantifying the degree of separation of samples in multivariate space, have been applied to date. Additional approaches, however (see 'Emerging methods for analysing field biological data' below), will assist in the further refinement of these site-specific WQGs.

Case study 2: Argyle diamond mine

The Argyle diamond mine is located about 550 km southwest of Darwin in northern Western Australia (Kimberley region). This region also experiences a wet–dry tropical climate, with an average annual rainfall of approximately 625 mm, most of which falls between December and March. The mine lies at the headwaters of two seasonal streams, Limestone Creek and Smoke Creek, to which mine seepage waters, in which $MgSO_4$ is the dominant solute, are discharged. During post-wet season recessional flow periods, electrical conductivities (ECs) associated with mine water discharges just downstream of the mine site are ~3,000 μS/cm and 550 μS/cm in Limestone and Smoke creeks, respectively, compared with a natural background of ~150–250 μS/cm. To assess the environmental effects of these high EC seepage waters, comprehensive laboratory- and field-based chemical and biological assessments were undertaken (Humphrey et al. 2008; van Dam et al. 2008). Both the laboratory and field data were used to inform the derivation of a site-specific WQG and WQO for EC for the site. Strong relationships between EC and Mg (r^2=0.764) and EC and SO_4 (r^2=0.770) enabled EC to be used as an indicator of $MgSO_4$.

Local toxicity data

The laboratory studies comprised a detailed toxicity testing program, using local and regional species, whose general aims were to (1) identify discharges of most concern, and (2) quantify the toxicity of key discharge waters in order to predict their ecological risk. The toxicity of seepage water was assessed in local receiving water from an un-impacted tributary of Limestone Creek using seven tropical freshwater species (a microalga, a macrophyte, two cladocerans, two cnidarians and a fish). Two of the species (one each of the cladoceran and cnidarian species) were collected locally, while the remaining five, although not collected locally, were known to occur in the region. With the exception of the aquatic plant species, all species were acclimated in the local control water for up to 2 weeks prior to the testing, to ensure acceptable health and performance in this water. Test environmental conditions were consistent with the regional tropical climate (i.e. 27 °C, 12-h/12-h photoperiod).

By integrating information on the toxicity of the seepage water, the concentrations of, and existing generic WQGs for, key constituents in the seepage water, and available relevant metal toxicity data, the key toxic constituent was identified as being $MgSO_4$, although minor contributions to toxicity from several other toxicants could not be fully discounted. Consequently, using the SSD approach, a laboratory-based 95 % species protection WQG (±95 % confidence limits) for EC (as an indicator of $MgSO_4$) of 280 μS/cm (240–520) was derived. Comparing this value with measured EC at the compliance points in the two creeks that receive mine seepage waters suggested a high likelihood of significant ecological risks (95 % exceedance of the WQG) in Limestone Creek, but low ecological risks (2 % exceedance of the WQG) in Smoke Creek. The laboratory toxicity data were then compared to, and integrated with, the field data, as described below.

Local field biological data

The field aquatic surveys gathered phytoplankton, zooplankton, macroinvertebrate and fish community data, together with accompanying water quality and environmental data, across eight to 16 mine-exposed sites and five to 13 reference sites, over the late wet/early dry seasons of 2006, 2007 and 2008 (Humphrey et al. 2008; van Dam et al. 2008). These surveys were designed to detect and quantify the impact of mine discharges on biota of the streams receiving seepage water by comparing assemblages of mine-exposed and reference sites.

The field data showed mine-related effects for all the taxa groups assessed except the fish, with the effects typically more pronounced in Limestone Creek than Smoke Creek. Some effects were observed in upper Smoke Creek, nearer the mine, but sites in lower Smoke Creek, where there was dilution by un-impacted tributaries, and EC was ≤250 μS/cm, were similar to reference sites. Effects were most marked for phytoplankton and zooplankton. Enhancement of growth was observed for phytoplankton at sites close to the mine site, most likely attributable to nitrate. Otherwise, significant impairment was observed for major zooplankton groups, the protists and microcrustaceans, most likely attributable to EC. Subtle mine-related effects were evident in macroinvertebrate communities, the next higher trophic and taxonomic level.

The effects upon macroinvertebrates were most evident as alterations to the structure of the communities (i.e. shifts in the abundance rankings of the different taxa), although one or two taxa appeared to be significantly impaired at the mine-exposed sites. In particular, a family of mayflies, Leptophlebiidae, was absent from virtually all exposed sites in Limestone and upper Smoke Creeks. Plots of EC against abundance of leptophlebiid mayfly nymphs showed a strong threshold effect of increasing EC and leptophlebiid mayfly absence (Fig. 4), with nymphs being absent from sites when EC exceeded 200–300 µS/cm.

To complement the various multivariate analyses, a community SSD (in the form of a cumulative distribution function) was constructed using presence–absence data from the field surveys (Fig. 5). Field-based (community) SSDs have been used previously to derive environmental quality guidelines for both waters and sediments (Kwok et al. 2008; Cormier et al. 2009). Recently, a comprehensive formal methodology for deriving environmental quality guidelines using field-based SSDs has been proposed (Cormier et al. 2013). This method will hopefully encourage further applications of field-based SSDs.

For the community SSD, the upper-most EC at which each taxon was reported to occur was assumed to represent that taxon's upper EC tolerance, referred to by Cormier et al. (2013) as the 'extirpation concentration' (i.e. the concentration that results in the depletion of a population to the point that it is no longer a viable resource or is unlikely to fulfil its function in the ecosystem). Although extirpation concentrations are less conservative than low/nil effect estimates (e.g. EC10s) derived from concentration–abundance relationships, they represent useful measures of effects since it is obvious that an adverse effect has occurred when a taxon is lost from an ecosystem (Cormier et al. 2013). In keeping with the methodology used to derive WQGs from laboratory-based SSDs, a 95 % species protection level was selected for the derivation of a WQG from the community SSD. The resultant WQG was approximately 200 µS/cm (rounded to two significant figures), which was consistent with the laboratory-based WQG of 280 µS/cm. Thus, information on natural background concentrations, laboratory toxicity and field biological effects indicated a WQG to provide full protection of the aquatic ecosystem would lie between 200 and 300 µS/cm.

As noted above, in Australia and New Zealand, WQOs represent agreed targets for water quality based on the WQGs and other inputs such as additional scientific data and social, economic or political imperatives. Notwithstanding the strong agreement between the laboratory- and field-based SSDs, the field studies showed that while some biological communities were altered, these changes were quite subtle. The receiving water ecosystems were still intact despite the altered water quality, and continued to sustain important environmental values and provide important ecosystem services including visual, social and recreational amenity. Moreover, there were few observations in the field of impacts to habitat (e.g. degradation of riparian vegetation, mine-derived precipitates on the stream bed, or excessive growth of filamentous algae), while the absence of impacts on fish communities indicated that the aquatic food webs were sufficiently intact to sustain healthy fish populations. Fishes are a resource that provides significant amenity as a food source to resident Aboriginal communities of the region.

Consequently, the collective field effects data provided technical information that would support and contribute to the

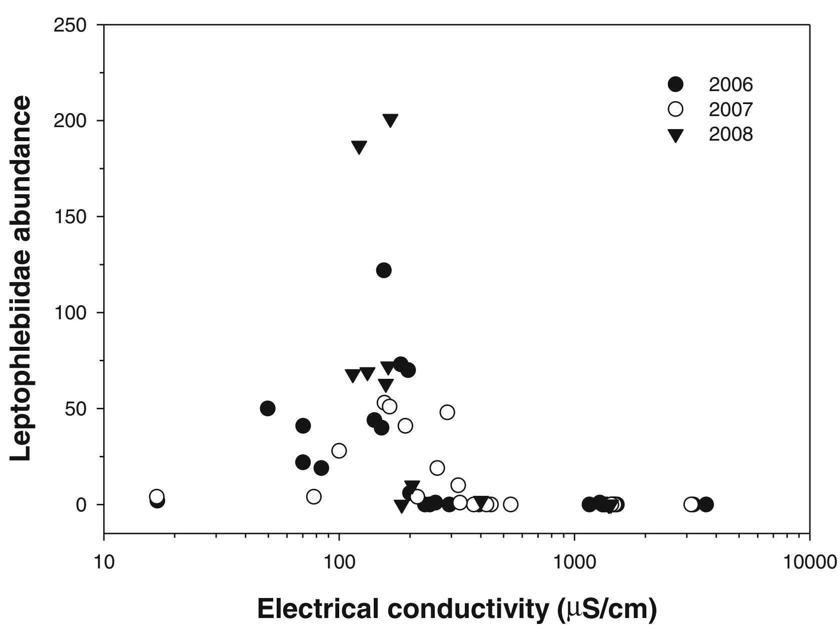

Fig. 4 Relationship between leptophlebiid nymph abundance and electrical conductivity (log scale) of surface waters at Argyle diamond mine sites for 2006, 2007 and 2008 sampling

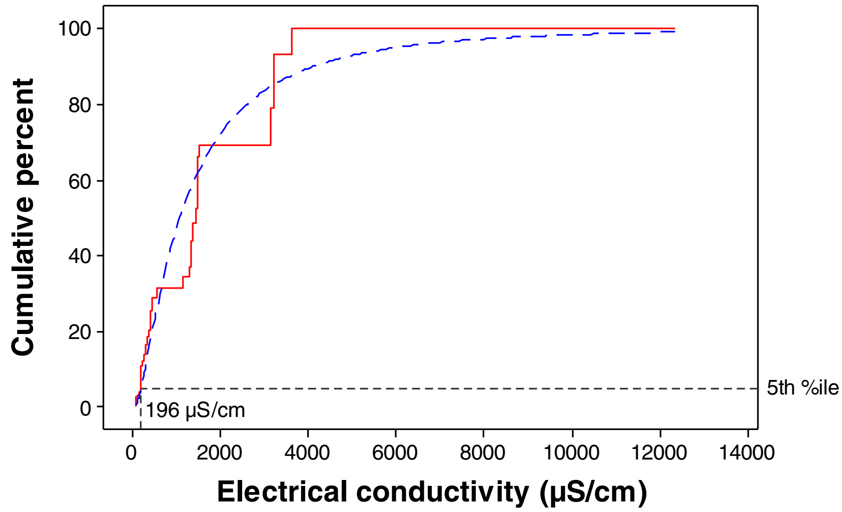

Fig. 5 Empirical (*solid line*) and fitted (*broken line*; lognormal distribution) cumulative distribution functions based on extirpation concentrations (upper electrical conductivity tolerances) for all taxa sampled in the 2006, 2007 and 2008 Argyle diamond mine field surveys (n=532). The *dotted line* at the 5th percentile indicates the 5 % hazardous concentration

development of a site-specific WQO. Specifically, the field assessments indicated that the key values of the receiving waters would be maintained providing mine water discharges did not lead to stream water quality at the compliance point worse than that observed in the 2006–2008 period over which the field studies were conducted. Thus, this was proposed as the WQO and the proposed framework to assess the WQO is described below.

Because flow in Limestone Creek is highest in the summer (December–April) wet season, receding in the ensuing dry season months, while mine discharges contribute a reasonably similar quantity and quality of seepage waters throughout the year, mine-related EC in the receiving waters varies seasonally. Analysis of the discharge–EC relationship indicated that as daily discharge increased during the wet season, EC declined as a result of dilution. Thus, to assess for any changes in EC, it was necessary to account for the effect of daily stream discharge. Figure 6 shows the quadratic relationship between daily discharge and average daily EC at the compliance point over the period the biological studies were undertaken. Assessment of change using this model can be performed at any frequency. For example, newly acquired or accruing median daily EC data can be compared to this model at the relevant daily discharge value to determine if they lie below the upper 95 % prediction interval (PIs) of the "reference" water quality distribution. In addition, if the discharge–EC regression relationship for a full future wet season does not fall within the 95 % prediction intervals of the "reference" relationship then this would indicate that water quality has deteriorated beyond that observed during the "reference" period. Although the possible WQO and associated assessment framework described here are yet to be formally agreed by stakeholders for implementation, the example illustrates the approach promoted by (ANZECC/ARMCANZ 2000) for such target setting and assessment.

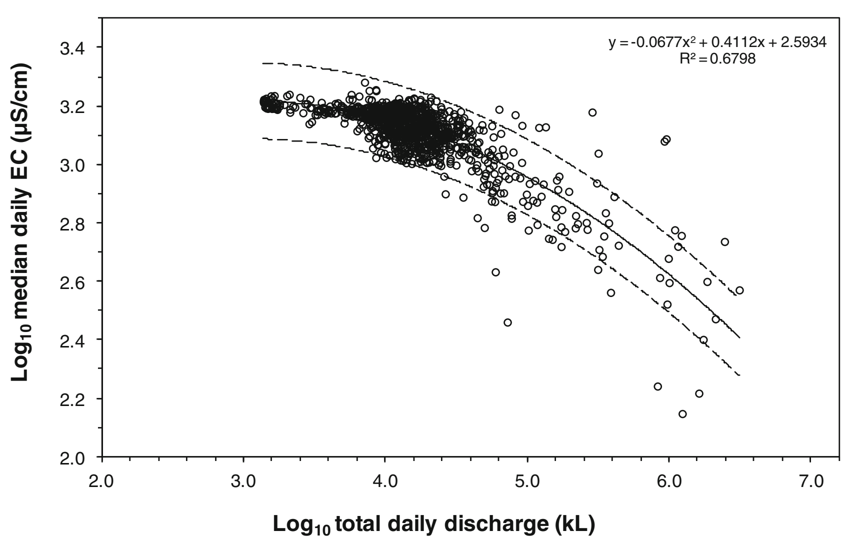

Fig. 6 Relationship between $\log_{10}$ median daily electrical conductivity and $\log_{10}$ total daily discharge using telemetered (15-min interval) data (n=1,096) from Argyle diamond mine gauging station for the years 2006–2008. The quadratic regression line is indicated by the unbroken line and 95 % prediction intervals indicated by the *broken lines*. The model can be used to monitor for changes in water quality from the current state (see main text for details)

Emerging methods for analysing field biological data

Apart from the existing field-based methods such as described in the two case studies, there have been several recently-published methods that show great promise for assessing and detecting thresholds of community change along toxicant gradients in the field and, subsequently, for deriving water or sediment quality guidelines. These methods include Threshold Indicator Taxa Analysis (TITAN), Gradient Forests and Non-linear canonical analysis of principal coordinates (NCAP), each of which are briefly described.

The TITAN method (Baker and King 2010) is based on the indicator value scores developed by Dufrêne and Legendre (1997). TITAN has been used to detect thresholds along gradients for a number of chemical stressors, including EC (Bernhardt et al. 2012) and total phosphorus in aquatic systems (Baker and King 2010), and for atmospheric nitrogen (Payne et al. 2013). The method integrates occurrence, abundance and directionality of taxa responses, to produce change points (thresholds) for individual species and the community as a whole. It does this for both species disappearing and species that are appearing along an environmental gradient. The method uses bootstrap sampling to assess the uncertainty of the change point and thereby estimates confidence limits around the value. The TITAN method has appeal in that it can identify community level change at environmental thresholds, and it can also identify which species are appreciably influencing the change. The method is limited to using only one key environmental predictor and, as a consequence, other influencing environmental predictors may be overlooked.

The Gradient Forests method (Ellis et al. 2012) uses random (regression tree) forests, which are grown for each individual species. Each random forest consists of a group of regression trees that repeatedly split the observations into partitions. The splitting occurs at certain values of an environmental predictor and produces functions that represent the compositional turnover along each environmental gradient. Gradient Forests has recently been used to assess benthic community changes in the far northern Great Barrier Reef in relation to 29 physical, chemical and biological variables (Ellis et al. 2012). Like TITAN, Gradient Forests shows promise as a tool for deriving field-based WQGs because it can identify changes along an environmental gradient, and can identify which species are changing at certain concentrations. It also has the advantage of being able to do this for any number of environmental parameters and can determine which parameter is the most important. Whilst the method does not produce a single change point value, it is clear that one may be inferred from the outputs produced by the analysis. The method also does not provide confidence limits around the estimates.

The NCAP method (Millar et al. 2005) is an extension of the CAP analysis (Anderson and Willis 2003) and uses a link function that can be a model of any particular form (e.g. non-linear: exponential decay, sigmoidal, etc.). Whilst NCAP has only been used to date to assess ecological responses associated with habitat changes, it has clear application for assessing chemical contamination gradients. The NCAP method uses distance-based dissimilarity measures and conducts Principle Coordinate Analysis. A non-linear gradient that maximises the canonical correlation with the principal coordinates is then defined. The significance of the fit of the non-linear gradient is determined by a randomisation procedure and bootstrapping is used to determine confidence limits of parameters for the non-linear model. This method is attractive because logistic models, which are often used to model concentration–response relationships, can be fitted to community datasets to derive toxicity estimates.

The usefulness of the above methods for deriving site-specific (and regional) WQGs based on field community data will take some time to assess. One potential challenge with the effective use of such methods is the ability to collect enough samples across a sufficiently large environmental gradient to enable a robust estimate of the threshold concentration. Further, even if the potential of these methods for determining thresholds of community change to toxicant exposure is realised, further consideration will be required as to how such information can be used to derive WQGs.

Summary and conclusions

Whilst requiring substantial data and effort to develop, site-specific WQGs provide greater confidence in ensuring an appropriate level of environmental protection than is possible from the use of generic WQGs. This paper has outlined key aspects of the current guidance in Australia and New Zealand for deriving site-specific WQGs (and their possible modification to WQOs), and illustrated the application of three approaches with case studies. Overall, the current guidance is consistent with that promoted by other countries and, as such, the examples are also relevant outside of Australia and New Zealand.

To assist those who are considering following this approach in their jurisdictions, we have summarised below several key lessons from our experiences in deriving site-specific WQGs, many of which are evident in the examples above.

Understand the issue This is no different to the problem formulation phase of risk assessment. An in-depth understanding of the toxicant(s) of concern and the water quality characteristics at the site of interest is necessary in order to determine whether there is a need to derive site-specific WQGs and, subsequently, to know what are the key local factors that the WQGs need to take account of. Aspects to consider include: how many and what types of toxicants are present; what are the characteristics of the key toxicant pathways; what are the ecosystems that need to be protected and in what condition are they; are there specific species or communities that warrant special consideration; what environmental (including climatic) factors may affect the bioavailability and toxicity of key toxicants; and what level of protection does the community expect.

Appropriateness of objectives and of methods The knowledge subsequently acquired should be used to formulate clear study objectives that are relevant to, and will address, the issue. This should then flow on to the methods chosen to assess the issue, such that they are appropriate for achieving the objectives. If it is agreed that site-specific WQGs are needed, careful consideration needs to be given to which methods are the most appropriate, and how important local environmental factors can be incorporated into the assessment.

Understand the guidance documents, but be prepared to adapt the principles for local conditions The ANZECC/ARMCANZ (2000) water quality guidelines and the corresponding guidance documents used in other countries are a key resource. They provide much of the guidance that is required to determine the most appropriate method(s) for deriving site-specific WQGs. However, many water quality issues will present challenges that are not necessarily captured by the existing guidance. Thus, it is often necessary to think beyond the guidance in order to design a locally specific program of work that is best fit for the purpose. This aspect has been highlighted above by the Mg pulse exposure WQGs for the Ranger uranium mine and the proposed EC WQO for Argyle diamond mine.

The emerging methods for data analysis that have been presented illustrate that this is a continually evolving field. The application of such methods should be considered, noting they are not yet contained in any formal jurisdictional guidance, which is often, by its nature, many years behind the evolving state of the art.

The strengths of integrated assessment and multiple lines of evidence Confidence in site-specific WQGs increases markedly if they are supported by multiple lines of evidence. Indeed, as noted above, site-specific WQGs based on laboratory toxicity data alone may not provide a sufficient level of confidence. Consequently, it is recommended that data from field studies are used to confirm that the WQGs are indeed appropriately protective. Subsequently, more recently acquired (field or laboratory) data should then be used to refine site-specific WQGs where possible. This approach has the additional benefit of enabling the refinement of monitoring and regulatory compliance programs over time.

Transparency Transparency in communicating and justifying key decisions, assumptions and approaches, and the associated uncertainties in the derived WQGs, is critical, especially when working outside existing guidance frameworks.

Quality Given the importance of site-specific WQGs for protecting aquatic ecosystems from toxicant impacts, there is a need to clearly demonstrate quality data and associated analysis and interpretation. It is recommended that a peer review process is used to verify the quality of a water quality assessment and/or site-specific WQG derivation.

The guidance summarised and illustrated through case studies in this paper provides a strong foundation to assist others in the derivation of site-specific WQGs.

Acknowledgments We would like to thank Argyle Diamonds P/L for approving the inclusion of the Argyle case study in this paper. We also acknowledge the staff of the Environmental Research Institute of the Supervising Scientist who have contributed to the work that was included in the case studies.

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