U.S. ENVIRONMENTAL PROTECTION AGENCY

Best Practices for Submitting Metals Data to the Water Quality eXchange (WQX)

Created in collaboration with the U.S. Environmental Protection Agency, the U.S. Geological Survey and Water Quality eXchange state partners

Executive Summary

Data submitted via WQX is published through the Water Quality Portal and made available with USGS, USDA and other state, tribal, territory, academic, and volunteer partners. The goal of the WQX Metals Best Practices Guide is to increase the quality of metals data records in WQX by making it easier for data providers to capture metadata elements, increasing consistency of metadata elements utilized, and removing confusion and ambiguity for secondary data users. This guide outlines how WQX data submitters can capture a complete metals record which includes: a metals characteristic, sample fraction, and analytical method. It is preferential for organizations to publish their data using a national analytical method to enhance data reuse and comparability with other datasets available through the Water Quality Portal. This document is a direct product of the WQX Metals Quality Assurance Workgroup, comprised of representatives from EPA, USGS, external stakeholders, and several states. The Metals Quality Assurance team has included details regarding metadata element capture decision points, how to propose new metals characteristics for use in WQX, and commonly reported metal records combinations. This guidance does not require any new metadata to be submitted to WQX but does advise data submitters to make adjustments to characteristic names and new characteristic name proposals.

To learn about best practices for capturing Nutrient data and metadata elements see the WQX Nutrient Best Practices Guide at https://www.epa.gov/waterdata/wqx-nutrients-best-practices-guide

Introduction

Metals data are collected, analyzed, and then published to WQX by hundreds of organizations throughout the country. Each of those organizations have unique projects and purposes for which they are collecting valuable and high-quality data. It is natural that each of those organizations store metals data with varying metadata elements and define metadata terms for their own analysis purposes. Likewise, data collected by the organization may have metadata qualities that can be assumed and thus not captured in the dataset. However, once the data is reported nationally, those metadata nuances that can be assumed at an organizational level, can no longer be assumed at the national level. By clarifying ambiguous terms, providing user guidance, and improving WQX submission requirements, the WQX metals data can be captured at such detail to facilitate secondary data usage.

The Water Quality eXchange (WQX) Metals Best Practices Guide was created to assist organizations in submitting metals data to WQX, by promoting consistency when capturing metadata and removing confusion and ambiguity for secondary data users. This document is a direct product of the WQX Metals Quality Assurance Workgroup, comprised of representatives from EPA, USGS, external stakeholders, and several states. The QA Workgroup addressed three areas of concern for metal characteristics: (1) Method Speciation, Ions and Sample Fraction, (2) National Analytical Methods, and (3) Metal Results. This Guide is designed to be used with WQX version 2.0, although some of these practices address elements that may become required in WQX 3.0 (scheduled for release in 2018-2019). It is recommended to adopt them now in anticipation of their inclusion in 3.0.

Documenting Method Speciation, Ions and Sample Fraction for Metals Characteristics

Speciation

Metals are only ever reported as a single speciation, thus the workgroup determined that method speciation is a nonessential metadata element and should not be a required data element. For example: Aluminum is always reported

"as Al", thus there is no need to require data submitters to report metadata that can be reasonably assumed. Ionic forms, which are sometimes referred to as the speciation of a metal, are identified as the ionic form in the characteristic name, such as Arsenic(III) or Chromium(VI), as described below.

Ions

Metals are found in multiple ionic forms in nature, which becomes important when assessing bioavailability of the metal. WQX needs to allow for the reporting of these ionic variants, such as Chromium(VI) and Chromium(III). After review of the current WQX metals characteristic list and the EPA Substance Registry System (SRS), the team determined the format for establishing new metal ion characteristics will be the metal name followed by the ion numeric value shown in the Chromium example above. When requesting ionic forms of metals to be added to the WQX characteristics allowable value list, please do so using the preferred format.

Sample Fraction

The sample fractions of "Total" and "Dissolved" when used with metals indicate an unfiltered and filtered sample, respectively. The workgroup found that the use of "Total" and "Dissolved" for metals is not ambiguous because only one speciation can be reported for each characteristic, eliminating the possibility that "Total" could indicate the sum of all forms. Total recoverable on the other hand, are the metals solubilized by digestion with strong solutions of mineral acids and is sometimes incorrectly used synonymously with Total metals. Please check with your lab to ensure you are recording the correct sample fraction.

NOTE: To capture filter pore size in a data submission, please capture the information in the Result Comment metadata element.

National Analytical Methods

The table below was created by the QA Workgroup to show common combinations of the WQX metadata elements, characteristic, sample fraction, and national methods, needed for a complete metals result.

Referencing a national method under the laboratory analysis method metadata element improves data consistency. And although WQX does allow organizations to create unique Method IDs, this option is primarily for cases when the method has not yet been captured in the domain value list. Organizations should map their lab analytical methods to an existing WQX lab analytical method if at all possible. Optimally, the laboratory analyzes and reports data using a recognized national method such as APHA or USEPA (captured in the WQX metadata element "method context").

If the lab is using a method or SOP equivalent to a recognized national method such as USEPA, APHA Standard Methods, ASTM, etc., report the recognized national method. If you cannot map your analytical method to a national method, and must create a custom method, it is not recommended to use words like "QAPP" or "UNKNOWN" in the method ID. These types of method IDs require a secondary data user to find documents that are not readily available, and may result in the data not being used because the methods are inaccessible.. Analyzing and reporting data with national methods increases the archival and reuse value of the data because it can be more readily combined with data from other organizations.

The Analytical Methods listed in table 1 are the most commonly reported methods for each given metal characteristic. The methods are not directly applicable to each possible metal result combination with sample fraction. There exist less

frequently used methods included on the WQX allowable values list that are not listed in the table below. To look up these additional method IDs, go to https://www.epa.gov/waterdata/storage-and-retrieval-and-water-quality-exchange-domain-services-and-downloads#domain. The National Environmental Methods Index is another reference for analytical methods https://www.nemi.gov/home/. If the method used is a nationally recognized method or you are a node submitter, please email the STORET helpdesk (storet@epa.gov) with the NEMI information and your ID request. If the method is not in the table below, the domain value lists, or NEMI, then you should add a new analytical method by logging into WQX web. To add an analytical method in WQX Web, select "Domain Values" > "Edit Analytical Methods" > Identify the Org ID as the context > input the analytical method > Save.

Documenting Metal Results

A complete metal result contains a characteristic name, a result (or result detection condition) value and unit, a sample fraction, and analytical method. If reported as above or below a quantitation limit by the laboratory, the complete record will need to contain a detection limit type, value, and unit instead of a result value and unit.

Table 1: Metals Result Guidance at a Glance

Table 1: The table below shows each of the recommended characteristics to be reported to WQX, any previous WQX allowable values that are synonyms of the recommended characteristic, sample fractions which can be reported for those characteristics, and the most commonly reported national methods for those characteristics.

Preferred WQX Characteristic Name	Result Sample Fraction		Commonly-Reported Analytical Methods for Characteristic
Aluminum	Acid Soluble Bed Sediment Dissolved	Recoverable Total Total Recoverable	**USEPA**: 200.8, 200.7, 6010C, 1638, 6010B, 6010A, 6020A **APHA**: 3120 **HACH:** 10215
Antimony	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 6020, 1638, 6020A, 6010C, 6010B, 6020, 1620A, 6020B, 200.7
Arsenic (V) Former Synonyms – Arsenic ion (5+) & Arsenate	Total Dissolved		**USEPA**: 200.8, 6010C, 6020, 1638, 200.7, 6020A, 200.9, 6010B, 1632 **APHA**: 3114-B, 3113-B
Arsenic	Bed Sediment Dissolved Fixed Inorganic	Recoverable Total Total Recoverable	**USEPA**: 200.8, 6010C, 1638, 200.7, 6020A, 200.9, 6010B, 1632 **APHA**: 3114-B, 3113-B
Arsenic (III) Former Synonyms – Arsenic ion (3+) & Arsenite	Total Dissolved		**USEPA:** 1632 **APHA:** 3114-B
Barium	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 200.7, 6010C, 1638, 6010B, 6020A, 6020, 6010C, 1620A,
Beryllium	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 200.7, 1638, 6020, 6010B, 6020A, 1620A, 6020B

Preferred WQX Characteristic Name	Result Sample Fraction		Commonly-Reported Methods for Characteristic
Boron	Bed Sediment Dissolved Dissolved Fixed Inorganic	Recoverable Total Total Total Recoverable	**USEPA:** 200.7, 200.8, 6020, 6010C, 6010B, **APHA:** 2130
Cadmium	Bed Sediment Dissolved Pot. Dissolved	Recoverable Total Total Recoverable	**USEPA:** 200.8, 200.7, 6010C, 6020, 1638, 6020A, 6010B, 200.12, 200.9 **HACH**: 10217
Calcium	Total Dissolved		**USEPA:** 200.7, 6010C
Chromium	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 200.7, 6010C, 1638, 6020, 6020A, 200.12, 6010B, 1620(A) **APHA**: 3113-B **HACH**: 10218
Chromium(III)	Total Dissolved		**USEPA:** 6010C, 7199 **APHA:** 3500-CR(D)
Chromium(VI)	Dissolved Recoverable	Total Total Recoverable	**USEPA:** 218.6, 7199, 7196A, 200.8 **APHA:** 3500-CR(D), 3500-CR(B), 3500-CR(D)
Cobalt	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 200.7, 6020, 6020A, 6010C, 6010B
Copper	Bed Sediment Dissolved Pot. Dissolved	Recoverable Total Total Recoverable	**USEPA:** 200.8, 200.7, 6010C, 1638, 6020, 6010B, 200.9 **APHA:** 3120, 3500-CU(B) **HACH**: 10215
Ferrous ion	Total Dissolved		**HACH:** 8146
Gadolinium	Total Dissolved		**USEPA:** 200.8
Gold	Total Dissolved		**USEPA:** 200.7, 200.8
Iron	Bed Sediment Dissolved Recoverable		Total Total Recoverable
Lead	Bed Sediment Dissolved Pot. Dissolved Recoverable	Suspended Total Total Recoverable	**USEPA:** 200.7, 200.8, 1638, 6010B, 6010C, 6020A, 6010A **APHA:** 3111-B, 3120 **HACH**: 10215
Lithium	Bed Sediment Dissolved	Recoverable Total	**USEPA:** 200.8, 200.7, 6010C, 6020, 1638, 6010B, 6020A, 200.9, 200.12 **HACH:** 10216
Magnesium	Total Dissolved		**USEPA:** 200.7, 6010C
Manganese	Bed Sediment Dissolved Recoverable	Suspended Total Total Recoverable	**USEPA:** 200.8, 200.7, 6010B
Mercury	Bed Sediment Dissolved Recoverable	Suspended Total Total Recoverable	**USEPA:** 200.7, 200.8, 1638, 6010C, 6010B, 6020A, 1620(A), 6020 **APHA:** 3120, 3111-B
Molybdenum	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 245.1, 245.7, 1631, 1631E, 7471B, 7471A, 200.8, 7470A, 7473 **APHA:** 3112-B

Preferred WQX Characteristic Name	Result Sample Fraction		Commonly-Reported Methods for Characteristic
Nickel	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.7, 200.8, 6020, 6020A, 6010C, 6010B
Potassium	Bed Sediment Dissolved Free Available	Total Total Recoverable	**USEPA:** 200.7, 200.8, 6010B, 1638, 300.1 **APHA:** 3120, 3111-B
Selenium	Bed Sediment Dissolved Dissolved Pot. Dissolved Recoverable	Suspended Total Total Total Recoverable	**USEPA:** 200.8, 200.7, 6010C, 1638, 6020, 6020B, 6020A, 6010B, 200.9 **HACH:** 10220
Silver	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 6010C, 6020, 1638, 200.7, 6020A, 200.9, 6010B **APHA:** 3114-C, 3114-B, 3113-B
Sodium	Bed Sediment Dissolved Fixed Free Available	Total Total Recoverable Recoverable	**USEPA:** 200.7, 200.8, 6010B, 6020A, 273.1, **APHA:** 3120B, 3111-B
Strontium	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 200.7, 6020, 6010C, 1638, 6020A, 6010B, 200.9, 6020B
Thallium	Bed Sediment Dissolved	Total Total Recoverable	**USEPA:** 200.7, 200.8, 1638, 6010B, 6020,
Tin	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 1638, 6020, 6020A, 6010C, 200.7, 6010B, 6020B, 300.0
Titanium	Bed Sediment Dissolved	Total Total Recoverable	**USEPA:** 200.7, 200.8
Vanadium	Bed Sediment Dissolved Recoverable	Total Total Recoverable	**USEPA:** 200.8, 200.7
Zinc	Bed Sediment Dissolved Pot. Dissolved	Recoverable Total Total Recoverable	**USEPA:** 200.8, 200.7, 6010C, 6020. 6020A, 6010B, 6010C, 1620(A), 1638