Best Practices for Submitting Nutrient 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

June 2, 2017

Introduction

The Water Quality eXchange (WQX) Nutrient Best Practices Guide was created to guide organizations in submitting nutrient data to WQX and to address other metadata issues with data to support the submission of nutrient information. This guide was also created to make submitting nutrient datasets more user-friendly, promote consistency when submitting data and thus remove confusion and ambiguity for secondary data users. It was produced through a WQX Nutrient QA Workgroup comprised of representatives from EPA, USGS and several States which were also members of the STORET/WQX Users Group. The QA Workgroup addressed six areas of concern with respect to documenting nutrient data to improve its value for secondary users. These include (1) duplicate monitoring locations, (2) addressing duplicate or ambiguous nutrient characteristic names (synonyms) in WQX (3), how to correctly use the WQX elements "method speciation" and "sample fraction", (4) correctly submitting values above or below detection limits, (5) National analytical methods, and (6) how to submit a complete and unambiguous nutrient result. This Guide is designed to be used with the 2.0 version of WQX. Some of these practices will become required elements in WQX 3.0 (scheduled for release in 2018), so we encourage data submitters to address them now.

Monitoring location: standardization, organization, and management

A monitoring location in WQX is a single location where samples were collected and results were reported. The three core elements of the WQX data structure include: Projects, Monitoring Locations, and Activities & Results. Projects and Monitoring Locations must be submitted to WQX prior to the Activities & Results to ensure the results contain a valid monitoring location and not, for example, a misspelling of the same location. Similarly, data submitters are sometimes unaware that a monitoring location already exists in WQX, and submit a duplicate location. To avoid submitting duplicate locations and improve ability to detect changes for that location overtime, consider developing a Standard Operating Procedure (SOP) for managing the locations.

Best practices for managing and submitting monitoring locations to WQX:

- When collecting data, a GPS can be used to store existing monitoring locations. Locations can be programmed into a GPS to be used to determine whether a new location should be created or an existing station is representative of the same measurement while in the field.
- Develop a process for managing the master monitoring location list. The process/SOP should be shared with all individuals involved in sampling and data management. The responsibility of maintaining the list can be assigned to a staff person in the organization but each employee involved with the data should be aware of the process for creating a new monitoring location. The use of geospatial tools to query based on spatial location, can greatly aid in reconciliation of locations.
- Prior to submitting data to WQX, review the monitoring locations in the water quality portal to determine which locations have already been created for the collecting organization. To do so, go to the Water Quality Portal (WQP) at waterqualitydata.us and download the organization's locations. This will serve as a starting guide for identifying where the organization has sampled before, what monitoring locations need added to WQX, and whether there are duplicate monitoring locations.
- Monitoring locations can be very close to one another and not be representative of the same water quality. In these instances, add a new monitoring location with its corresponding metadata and explain the difference of the locations using the monitoring location description field.
- If the organization has duplicate locations in WQX, verify the locations with the internal master list or check previous data submissions. If duplicates exist, combine them by re-submitting corrected data from the duplicate location to the desired location and then delete the duplicate location and its associated data. **NOTE:** Once a location in WQX is deleted, all samples and results associated with the location will also be deleted.

- If the organization is collecting data for probabilistic monitoring locations, please include the additional project data elements under "Project Monitoring Location Weighting" in the Data Exchange Template . If the data are used for probabilistic monitoring and another project, multiple project IDs can be assigned to the result.

Consistently use the same characteristic names

The Nutrient QA Workgroup found users have submitted the same laboratory results under varying characteristic names over the years. For example, an organization might submit results using "Phosphorus-phosphate" one year and "Phosphorus" the next year, when both were collected and analyzed the same way. When initiating each data submission, it's good practice to download the organization's data from the WQP at waterqualitydata.us to find how results were previously reported. Verify the lab analyzed samples using the same methods, and that its appropriate to continue reporting the same way. The QA Workgroup identified many duplicate or synonymous names in the WQX nutrient characteristic list, including "Phosphate-Phosphorus" and "Phosphorus". These duplicate names were consolidated in Table 4, which lists the desired characteristic names and synonyms that previously existed in WQX. We encourage users to provide the preferred WQX characteristic names when submitting results. Use of the synonym names will return an error message for new submissions under WQX 3.0, although those names submitted under earlier WQX versions will be available for data retrieval in the WQP.

The column "Former WQX Characteristic Name(s) (Synonyms)" in table 4 contains nutrient Characteristic names that should no longer be used for reporting data to WQX. If your organization is reporting a Characteristic in the synonym list, please use the "Preferred WQX Characteristic Name" instead. When creating rules in a database for nutrient results, refer to this table to help create the allowable values lists for the database.

Documenting Method Speciation and Sample Fraction for Nutrient Characteristics

Have a discussion with the lab about the analyses they will complete, what exactly is measured with the methods (e.g. sum of all forms or an unfiltered sample), and the expectations of how the data will be reported to correctly document method speciation and sample fraction.

Method Speciation

The method speciation name, the WQX equivalent name to what people may call the result speciation, is the portion/component of the chemical measured in a sample. This distinction is important to document because some labs/methods will use one portion of the characteristic and thus report that portion of the original sample.

For example: Nitrate results can be reported "as Nitrate" (the molecular form, NO3 = 1 Nitrogen atom + 3 Oxygen atoms) or "as Nitrogen" (the elemental form, N = 1 Nitrogen atom). The Nitrogen atom accounts for 22.5% of the weight of a Nitrate molecule. The oxygen atoms account for the rest. So, the same amount of Nitrate in a single sample can be reported two ways--"Nitrate as N" or "Nitrate as NO3". The "Nitrate as N" value will be 22.5% of the "Nitrate as NO3." value. For example, 1 mg/L of Nitrate as N is the same as 4.5 mg/L Nitrate as NO3 for the same amount of Nitrate in a single sample.

The following equation demonstrates the concept in a conversion factor:

45mg/L Nitrate as NO3 X 0.225 = 10 mg/L Nitrate as N

This is why the U.S. EPA Drinking Water Maximum Contaminant Level (MCL) for Nitrate is expressed either as 10 mg/L of Nitrate as N or 45 mg/L of Nitrate as NO3. If the incorrect speciation is reported or no speciation is reported, the value can bias an analysis. All nutrients require speciation reporting, including Ammonia (NH3), Nitrite (NO2) and Orthophosphate (PO4). When submitting data to WQX, the user should not submit the same result in multiple speciations. This could result in an analyst or secondary user thinking two individual results were reported when in reality a conversion was performed on the original result value. The data analyst or secondary user will need to apply a conversion factor to obtain a different speciation than reported. The table below, shows the conversion factors that can be used for Ammonia, Ammonium, Nitrite, Nitrate, and Orthophosphate. **NOTE**: Subscript notation is not used in WQX so please capture speciation in the format shown in the WQX allowable value lists.

Characteristic	Reported Speciation	Multiply By	To obtain
Ammonia	as NH3	0.822	as N
Ammonium	as NH4	0.776	as N
Nitrite	as NO2	0.304	as N
Nitrate	as NO3	0.225	as N
Orthophosphate	as PO4	0.326	as P

Table 1: The above table shows the conversion factors for obtaining as N and as P values for commonly reported characteristics

For example, many environmental labs report nutrient data as:

Nitrate or

Nitrate as N

By reporting "Nitrate," they may mean they are reporting the molecular form, or "Nitrate as NO3", because they find it redundant to report "Nitrate as Nitrate." However, data users cannot be sure of the meaning unless it is documented. What if the results were really reported as "Nitrate as N?" If speciation is not clear, the data cannot be used with confidence.

This is why we encourage speciation to be reported, even if it seems redundant. We want to make sure data users know exactly what they are getting when they use this information. Make sure the lab reports nutrient results like this example:

Nitrate as NO3 or

Nitrate as N

Values can that are calculated from other analyses, such as inorganic nitrogen and the individual portions that comprise inorganic nitrogen can be submitted. See table 4, Nutrient Result Guidance at a Glance for help with reporting speciation for nutrient characteristics to WQX/STORET. This table contains all the possible speciations which can be reported for each preferred characteristic.

Sample Fraction

Filtration is the physical process used to separate the particulate and aqueous fractions of a water sample. Unfiltered results will include the amount of chemical associated with both the particulate and the aqueous fractions. Filtered results will include the amount of chemical associated with just the aqueous fraction. Knowledge of the filtration status of a sample is vital because filtered and unfiltered values for the same characteristic may be very different.

Water samples can be filtered in the field at the time of collection or in the laboratory prior to analysis. For some characteristics, the same laboratory method can be used on both a filtered and an unfiltered sample. As a result, a description of the laboratory method is not always a reliable determinant of filtration status. If there is any uncertainty, chemists in the laboratory and staff collecting the original samples should record filtration status.

The terms "filtered, field", "filtered, lab" and "unfiltered" are more precise, and therefore preferred, over "dissolved" and "total." In particular, "total" is ambiguous, because it has been used to represent two different concepts:

(1) the inclusion of multiple species, such as when ammonia and organic nitrogen are summed to give total Kjeldahl nitrogen, or when all dissolved phosphorus species are included in the determination of total dissolved phosphorus

(2) to represent an unfiltered sample. An example of a clear, unambiguous characteristic description is Total nitrogen mixed forms, water, filtered, field, milligrams per liter as N". (See table 2 below)

The "filtered, field" and "filtered, lab" values were created to unambiguously define where a sample was filtered. This distinction is not required for some nutrient analyses. However, particularly with ground water, the distinction is critical to use the data. Because WQX is a data standard that is used for all water data types, the allowable values were created to not only support surface water data but also ground water. To use these values properly, if a nutrient sample was filtered in the field, indicate "filtered, field", regardless if it was also filtered by the lab. If it was not filtered in the field, confirm with the lab whether or not the sample was lab filtered before analysis, "filtered, lab". If it was not filtered prior to the analysis describe the result as "unfiltered".

The Nitrogen, Phosphorus, and Kjeldahl Nitrogen characteristic names now include the terms "Total" and the forms in parentheses distinguishing the constituents included in the label "total". This should help users choose the correct characteristic name when submitting data and help data consumers understand exactly what they are getting. An example of a new characteristic name is "Total Nitrogen (mixed forms)". The QA Workgroup thought the best way to explain the intent of "Total" was to include its definition, "mixed forms", meaning **the sum of all forms** in the characteristic name. For more information on what is meant by "Total" see the sample fraction section of this document.

NOTE: To capture filter pore size in a data submission, please capture the information in the result comment data element.

Media	Characteristic	Method Speciation	Result Value	Result Unit	Result Sample Fraction	Analytical Method
Water	Total Nitrogen, mixed forms	as N	2.0	mg/L	Filtered, field	USEPA 351.1

Table 2: The table represents a complete nutrient that can be used for secondary analyses.

Correctly document censored data (i.e. data above or below Detection/Quantitation limit)

Detection condition is a way to document a result for which there is no numeric value (e.g. Below Quantitation Limit or Below Method Detection Limit). Sharing results which are below a detection or quantitation limit is equally as important as sharing results that have a specific value unqualified by the laboratory. Censored data, or detection condition data, provides data users with valuable information about water-quality conditions at that monitoring location, including conditions where very low concentrations occur. Without the censored data, an analyst may assume there were no results below the laboratory detection limit at the monitoring location, which will greatly impact basic statistics such as average concentration or percent of samples exceeding a criterion or threshold. Failing to use censored data will skew the analyses and decisions based on them.

To better ensure data are used in the correct context, make sure to provide censored data and use appropriate fields to document it as described below. Instead of using the result value field for censored data, use the WQX field "Result Detection Condition" to unambiguously identify values outside a method's limits of detection or quantification. WQX requires **either** the result **or** result detection condition to enforce data rules to ensure a complete record. Symbols such as <, >, *, ~, do not translate to a national data standard including WQX. Special characters can lead to misinterpreted by data users. Furthermore, when a censored value is submitted in the result value column, WQX cannot correctly check for a complete and valid record leading to data quality issues. Table 3 below shows that a result detection condition can be reported OR the result value, but not both (shown in red below). A result limit type, limit measure, and limit unit are optional if a result value is reported, but are required if the result is a result detection condition.

Characteristic Name	Result Detection Condition	Result Value	Result Unit	Result Detection/Quantitation Limit Type	Result Detection/Quantitation Limit Measure	Result Detection/Quantitation Limit Unit
Nitrite		4.46	mg/l	Method Detection Level	0.001	mg/l
Nitrogen-15		11.3	mg/l			
Ammonia-nitrogen		0.8022	mg/l			
Nitrate		6.2	mg/l			
Nitrite	Present Below Quantification Limit			Lower Quantitation Limit	0.50	mg/l
Nitrogen-15		10.3	mg/l			
Ammonia-nitrogen		1.0022	mg/l			
Nitrate	Not Detected			Method Detection Level	0.001	mg/l
Nitrite		5.46	mg/l			
Nitrogen-15		12.3	mg/l			

Table 3: The above table shows the WQX rule for capturing censored data. Either the Result Detection Condition or Result Value may be provided, but not both. If a censored value is reported, the corresponding detection limit and metadata must be submitted. Multiple detection limits may be reported with an individual result.

A value reported as below a laboratory detection limit does not mean the true concentration is zero or that the result is equal to the detection limit. For more information about the importance of censored data and its inclusion in data analyses, view the National Water Quality Monitoring Webinar and presentation slide deck at https://www.youtube.com/watch?v=azL7nFREZlg and https://acwi.gov/monitoring/webinars/nada-111516.pdf.

As demonstrated above, censored data is documented using the result detection condition element, the result detection/quantitation limit type element, result detection/quantitation limit measure element, and result detection/quantitation limit unit. WQX provides a list of allowable values for "Result Detection Condition" and "Result Detection/Quantitation limit type" which is available at https://www.epa.gov/waterdata/storage-and-retrieval-and-water-quality-exchange-domain-services-and-downloads#domain.

A review of the allowable value lists for result detection condition and result detection/quantitation limit type found there are ambiguous and inappropriate values in the lists. Allowable values such as “Water Quality Standard or Criteria” or “High Moisture” are data more appropriate for comment fields, and will be retired from the detection/quantitation allowable value lists available for future data submissions.

National Analytical Methods

The QA Workgroup created table 4 with common combinations of the WQX data elements needed for a complete nutrient result. The table shows the speciation and sample fraction metadata elements for each nutrient characteristic and the top-reported national methods for those characteristics.

Use of a national method for laboratory analysis improves data consistency. WQX does allow organizations to create unique Method IDs. This option is primarily for cases when the WQX Analysis Method domain value list does not contain a method. Organizations should map analytical methods to an existing WQX method if possible. Optimally, the laboratory will analyze and report data using a recognized national method (i.e. WQX data element “method context”) such as APHA or USEPA.

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, instead of creating a custom method. Creating new analytical methods in WQX that contain the words “QAPP” or “UNKNOWN”, are impediments to data reuse. These methods require the data user to find documents that are not readily available or perhaps to not use the data at all because the methods are inaccessible or will cost too much time and/or effort to verify.

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. An example is EPA 350.1 (Nitrogen as Ammonia, Colorimetric, Automated Phenate). Data is more likely to be used by data consumers and be comparable to other data if it is analyzed and documented using a national method.

The Analytical Methods listed in table 4 are the most commonly reported methods for each given nutrient characteristic. The methods are not directly applicable to each possible nutrient result combination of method speciation and sample fraction. There are additional, less frequently used methods included on the allowable values list that are not listed in the table below. To look up 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 below table, not in the domain value lists, or in NEMI, add a new method for the organization by logging into WQX web. To do so, in WQX Web select “Domain Values” > “Edit Analytical Methods” > Identify the Org ID as the context > input the analytical method > Save.

Documenting Nutrient Results

Nutrient data is collected, analyzed, and then shared 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 these organizations store nutrient data with varying metadata elements and define metadata terms for their own analysis purposes. Data collected for a particular purpose and analyzed by the same lab, using the same methods throughout time, will have metadata qualities that can be assumed. However, once the data is reported

nationally, those metadata nuances that can be assumed at an organization level, can no longer be assumed at the national level. By clarifying ambiguous terms, providing user guidance, and improving WQX submission requirements, the WQX nutrient data can be captured at such detail to facilitate secondary data usage.

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

Table 4 Nutrient Result Guidance at a Glance

Preferred WQX Characteristic Name	Former WQX Characteristic Name(s) (Synonyms)	Method Speciation	Result Sample Fraction	Top-Reported Methods for Preferred Characteristic
Ammonia	○ Ammonia Nitrogen ○ Nitrogen, ammonia (NH3)	as N or as NH3	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 350.1 **APHA:** 4500-NH3(C), 4500-NH3(E) **HACH**: 8155, 10023 **ASTM**: D6919-03, D6919-09 **LACHAT:** 10-107-06-3-D
Ammonium	NA	as N or as NH4	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**APHA:** 4500-NH3(F), NH3(H) **ASTM:** D6919-03
Inorganic nitrogen (NO2, NO3, & NH3)	○ Inorganic nitrogen (ammonia, nitrate and nitrite)	as N	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 300.0, 353.1, 353.2, 353.4, 354.1 **APHA**: 4500-NO3(E), 4500-NO3(F), 4500-NO3(H) **ASTM**: D3867-04, **USDOIS/USGS**: I-4545 **LACHAT**: 10-107-04-1-J
Nitrate + Nitrite	○ Inorganic nitrogen (nitrate and nitrite)	as N	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 353.2, 353.1, 353.4, 300.0, 300.1, 300.6, 354.1 **APHA**: 4500-NO3(F), 4500-NO3(I), 4110-C,4110B, 4500-NO3(B), 4500-NO3(E) **ASTM**: D3867-04 **LACHAT**: 10-107-04-1-C
Total Kjeldahl nitrogen (Organic N & NH3)	○ Kjeldahl nitrogen	as N	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA:** 351.2, 351.3(A), 351.3(B), 351.3(C), 351.1, 351.4, 350.1, 350.2, 350.3 **APHA:** 4500-NORG(B), 4500-NORG C, 4500 NORG D, 4500-NH3(C), 4500-NH3(D), 4500-NH3(G) **HACH:** 10242 **ASTM:** D3590(A) **LACHAT:** 10-107-06-2-M
Nitrate	NA	as N or as NO3	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 353.2, 353.1, 352.1, 300.1, 300.0 **APHA**: 4500-NO3(D), 4500-NO3(E), 4500-NO3(F), 4500-NO3(H), 4110-B **HACH**: 10020 **ASTM:** D3867-04, D3867-16 **USDOI/USGS**: I4545
Nitrite	NA	as N or as NO2	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 353.2, 300, 300.1, 354.1 **APHA**: 4500-NO3(E),4500-NO3(F), 4500-NO2(B) **ASTM**: D3867-04, D3867-16 **USDOI/USGS:** I-4545

Preferred WQX Characteristic Name	Former WQX Characteristic Name(s) (Synonyms)	Method Speciation	Result Sample Fraction	Top-Reported Methods for Preferred Characteristic
Total Nitrogen, mixed forms	○ Nitrogen ○ Nitrogen, mixed forms (NH3), (NH4), organic, (NO2) and (NO3) ○ Nutrient-nitrogen ○ Total Particulate Nitrogen (capture with "Total Nitrogen, mixed forms with sample fraction "Suspended")	as N	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 353.1, 353.2, 353.3, 440(S), 440(W) **APHA**: 4500-NORG(C), 4500-P(J), 4500-NO3(D), 4500-NO3(E) **LACHAT:** 10-107-04-1-C
Organic Nitrogen	○ NA	as N	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA:** 351.2, **APHA** 4500-NORG(B) **LACHAT**: 10-107-06-2E
Organic Phosphorus	○ Phosphorus, Particulate Organic (capture as "Organic Phosphorus" with sample fraction "Suspended")	as P	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 365.2 **APHA**: 4500-P(E)
Orthophosphate	○ Inorganic Phosphorus	as P or as PO4	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 365.1, 365.3, 365.2, 365.4, 300.1, 3,365.5 **APHA**: 4500-P(E) **HACH**: 8048 **LACHAT**: 10-115-01-1-A
Total Phosphorus, mixed forms	○ Phosphate-phosphorus ○ Phosphorus ○ Phosphorus (Total: PO4 & Organic Phosphorus)	as P or as PO4	○ Filtered, Lab ○ Filtered, Field ○ Unfiltered ○ Non-Filterable (Particle)	**USEPA**: 365.1, 365.4, 365.3, 365.2 **APHA**: 4500-P(E) **HACH**: 10210, 8190 **ASTM**: D515(B) **USDOI/USGS**: I-4650-03 **LACHAT**: 10-115-01-1-F
Soluble Reactive Phosphorus	NA	as P as PO4	○ Filtered, Lab ○ Filtered, Field	**USEPA**: 365.1 **APHA**: 4500-P(E)

Table 4: The table above shows each of the recommended characteristics to be reported to WQX, the previous WQX allowable values that are synonyms of the recommended characteristic, the method speciations and sample fractions which can be reported for those characteristics, and the most commonly reported national methods for those characteristics.