## Nitrogenous Data Are Not All Equal Lee Moores, Ph.D. (uek2@cdc.gov), OCHHA Published in the ATSDR Newsletter for Health Assessors June 2024

The multifarious nitrogen analyses conducted by laboratories can lead to confusion due to the similarity of the analysis's names; however, there are some major differences that potentially impact health assessments if not handled properly. The most commonly confused data sets are those when the chemical name appears as "analyte-nitrogen," such as nitrate-nitrogen or nitrite-nitrogen. These data show only the concentration of the nitrogen, not the ion. This type of analysis is requested for ecological assessments to quantify the total amount of bioavailable nitrogen in an ecosystem. Using these as concentrations for human health assessments will result in an erroneous and less protective assessment, because the units between the dataset and comparison values are not the same. To transform the data into a useful concentration one must revisit some general chemistry principles and utilize the equation:

[nitrogenous analyte] = [nitrogenous analyte-nitrogen] x 
$$\frac{MW_{nitrogenous analyte}}{MW_{nitrogen}}$$
 Equation 1

Where the brackets indicate a concentration unit, MW<sub>nitrogen</sub>, is the molecular weight of nitrogen, or 14.007 atomic mass units (amu), and MW<sub>nitrogenous analyte</sub> is the molecular weight for the analyte in question. For example, if given a data set where the measured concentration of nitrate-nitrogen is 1.45 mg/L then the equivalent concentration in nitrate would be

1.45 mg nitrate-nitrogen/L x 
$$\frac{62.005}{14.007}$$
 = 4.53 mg nitrate /L Equation 2

And here with the same measured concentration as nitrite-nitrogen

1.45 mg nitrate-nitrogen/L x 
$$\frac{46.006}{14.007}$$
 = 4.76 mg nitrite /L Equation 3

Demonstrating the difference between the two analytes' molecular weights will result in a different concentration. Caution must be exercised to ensure the appropriate analyte is chosen.

Other times the nitrogen oxyanion data, for nitrate and nitrite, are presented as a sum because of the short sample holding time of 48 hours. Unfortunately, with only this information the interpretation of the potential hazard is greatly hampered. Nitrite is more toxic than nitrate, with minimal risk levels of 0.1 and 4.0 mg/kg/day, respectively. When concentrations are reported as nitrate and nitrite combined, the health protective approach would therefore be to assume all the combined data are from nitrite. If this approach would require further investigation, only additional sampling can be recommended where the data for the two ions

are determined individually. However, this will be difficult, often insurmountably so, given the logistics of taking a sample, shipping to a laboratory, and determining the nitrate and nitrite concentrations in less than 48 hours.

Health assessors should not use EPA's nitrate RfD of 1.6 mg/kg/day as this value only represents the nitrogen portion of the nitrate ion. Instead, if data are reported as nitrate-nitrogen, health assessors should convert the values to nitrate concentrations and use ATSDR's MRL (4 mg/kg/day).

There are other analyses for nitrogen containing data as well that should be questioned prior to making assumptions. Total nitrogen, a sum of ammonia, nitrite, nitrate, and organic nitrogen (e.g., amino acids, proteins, etc.) and Total Kjeldahl Nitrogen, a sum of ammonia and organic nitrogen, are two such analyses. These are not frequently encountered for environmental samples.

Equation 1 alt text (> 120 spaces)

Nitrogenous analyte concentration equals nitrogenous analyte-nitrogen concentration times the molecular weight of nitrogenous analyte divided by molecular weight nitrogen

Equation 2 alt text (< 120 spaces)

1.45 milligram nitrate-nitrogen per liter times 62.005 divided by 14.007 equals 4.53 milligrams nitrate per liter

Equation 3 alt text (< 120 spaces)

1.45 milligram nitrate-nitrogen per liter times 46.006 divided by 14.007 equals 4.76 milligrams nitrite per liter