Statistical Evaluations of Iron and Nitrate Influence on RDX Reduction

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The influence of iron on RDX destruction has been previously investigated in theoretical settings and bench-scale tests by various practitioners. The following is a summary of a statistical and mathematical assessment of this relationship using geochemical data from an ongoing groundwater remediation effort at the Iowa Army Ammunition Plant (IAAAP). IAAAP, which began production in 1941 and is still in operation, occupies approximately 19,000 acres adjacent to the town of Middletown in Des Moines County, Iowa. The past munitions production at IAAAP has resulted in contamination of soil and groundwater and discharge of wastewater containing explosives, such as RDX, and explosives by-products to surface water. Several focus areas at IAAAP are currently undergoing RDX bioreduction via the addition of high fructose corn syrup (HFCS). The reduced environment appears to mobilize the mineral-phase iron that was previously hypothesized to play a role in RDX abiotic treatment, which complements the well-accepted biotic treatment under these conditions. In order to better understand the overall in-situ process and focus future sampling activities on relevant parameters, groundwater monitoring results were analyzed to determine if correlations exist between RDX and other geochemical analytes. Initial data analyses included the calculation of Pearson correlation coefficients (linear regression) and the multi-variate Principle Component Analysis (PCA). In concert, these statistical methods begin to highlight analytes that show evidence of interdependence.

Rather than compare multiple focus areas at the site, this study examines the results from one particular area, L800 South, to illustrate the potential uses and difficulties associated with these statistical approaches. At L800-S, PCA results indicate that Total Organic Carbon (TOC) and Oxidation-Reduction Potential (ORP) show no strong correlation with RDX or its degradation products. The primary PCA eigenvectors indicate that DNX, MNX, dissolved oxygen, alkalinity, CO_2, total iron, and sulfate are all inter-related, as are RDX, TNX, nitrate, and methane. DNX and MNX show an inverse relation to the total iron concentration, which is interpreted as Fe(II) since Fe(III) is considered insoluble at neutral pHs. RDX shows an inverse relation to nitrate, while TNX is directly proportional. However, Pearson correlation coefficients indicate that RDX correlates significantly with only MNX, sulfate, and methane. This discrepancy between the two statistical methods indicates that simple linear regressions may not sufficiently take into consideration the complex multi-component inter-relations occurring at many sites. Both linear correlation analysis and PCA indicate that there is no single compound solely related to RDX and its degradation products which should be monitored as a strong indicator of remedial progress. Rather, both PCA and Pearson correlations results suggest that complex, site-specific, multi-parameter correlations exist and should be considered during remedial and monitoring activities.

Using well-established statistical techniques such as basic linear relations and PCA, complex interrelations between various chemicals of concern and geochemical parameters, as well as un-related or un-important species, can be established. Analogous statistical analyses at other sites can be used as a tool to eliminate superfluous sampling and focus future treatment and sampling efforts. Thus, project resources can be directed in the most productive and cost-effective manner.