Incorporating Transformation Products into Models of the Environmental Fate of Insensitive Munition Constituents

Paul G. Tratnyek (tratnyek@ohsu.edu) and
Tifany L. Torralba-Sanchez (Oregon Health & Science University, Portland, OR)
Eric J. Bylaska (Pacific Northwest National Laboratory, Richland, Washington)
Jalal Hawari (University of Montréal-Ecole Polytechnique, Montréal, QC)
Billy E. Johnson (U.S. Army Engineering Research and Development Center, Vicksburg, MS)

Background/Objectives. To provide a complete assessment of the potential environmental impacts of insensitive munitions constituents (IMCs), it is necessary to consider their *transformation products*. Transformation of the highest priority IMCs (DNAN and NTO) has recently been subjected to considerable study, but little is known about their transformation products, and even less is known about the fate and effects of these products. Data on the environmental fate determining properties of IMC degradation products are limited and methods for estimating these properties have not been validated for compounds of this type.

The overall goal of this new SERDP project (ER-2725) is to lay the foundation for comprehensive assessment of the fate and effects of IMC degradation products on training ranges and other DoD sites. The scope includes three major research objectives: (*i*) determination of IMC transformation pathways and products, (*ii*) determination of the fate determining properties of IMC transformation products, and (*iii*) development of models that describe the fate and transport of IMC transformation products. All of these results will be used to extend the reactive-transport model used by DoD training site managers (Training Range Environmental Evaluation and Characterization System [TREECS]) to include transformation and transformation products of IMCs.

Approach/Activities. The experimental aspects of this his study are focused on DNAN and NTO, but the models to be developed will accommodate a wide range of IMC parent compounds and daughter projects. The scope includes all of the fate-determining processes (volatilization, sorption, etc.), but with emphasis on transformation, the relative rates of competing transformation pathways, and the resulting variation in intermediate/products concentrations as a function of space and time. Batch experiments will be performed using environmentally-relevant materials to characterize transformation products and to measure fate-determining properties of those transformation products. Models that explain and predict the degradation pathways/products will be developed from computational chemistry or structure-activity relationships and validated with experimental data. Kinetic, reactive-transport models will be developed using general and environmentally-specific software for numerical simulation.

Results/Lessons Learned. The results of this project have practical and general applications. The practical benefit of this work will be to enable DoD training site managers to include consideration of IMC transformation and products into the modeling they do for evaluation of exposure assessment scenarios, risk, remediation, etc. For this type of application, technology transfer will occur through integration directly into the TREECS. General applications of the results from this project will be through advancement of methods for prediction of transformation pathways, chemical properties, and reactive-transport models that could be adapted for assessing the environmental fate of other classes of contaminants.