Heuristic Numerical Modeling Study of LNAPL Depletion under Natural Conditions

Parisa Jourabchi (pjourabchi@golder.com) and Ian Hers (Golder Associates, Ltd., Vancouver, BC, Canada), Andrew Kirkman (BP Remediation Management, Naperville, IL, USA) Ulrich Mayer (University of British Columbia, Vancouver, BC, Canada) and John Wilson (Scissortail Environmental Solutions, Ada, OK, USA)

Background/Objectives. Natural source zone depletion (NSZD) is a significant process for LNAPL mass depletion and compositional change at many petroleum hydrocarbon-impacted sites. While much recent work has been done in the area of NSZD estimation through measurement methods, there has been less emphasis on development of predictive models for heuristic evaluations of processes and quantitative estimates of mass loss and compositional change. The relative importance of aerobic versus anaerobic processes, saturated and unsaturated zone conditions, the mechanisms controlling degassing and ebullition and key site factors are not well understood. While potentially highly useful, measurement data such as surface gas effluxes are potentially limited with respect to assessing seasonal variability and saturated zone processes. The objective of this study is to develop an improved mechanistic or process-based understanding of natural LNAPL depletion using the MIN3P-Dusty numerical model.

Approach/Activities. A detailed conceptual site model was developed based on a literature review and our understanding of relevant processes. The key factors affecting NSZD rates are identified including the physical-chemical-biological properties of the LNAPL components, the redox reaction pathways, the LNAPL distribution relative to the water table, the LNAPL saturation and extent, and vadose zone soil physical properties. Properties and biodegradation rates depend on LNAPL composition, with less information available for heavier molecular weight hydrocarbons. The concepts of direct outgassing from LNAPL, degassing from the water phase, and ebullition are described together with available data and implications for modeling approaches. The MIN3P-Dusty model has significant capabilities for multi-dimensional simulation of natural and enhanced LNAPL depletion and compositional change from biodegradation, volatilization and dissolution using a process-based multicomponent modeling approach. For purposes of this project, the model is used heuristically to understand the influence of key factors, and to identify insights as well as potential gaps in understanding of processes and model capabilities. The results of numerical model simulations are also compared to the mass loss estimates predicted using the Vadose Zone Biodegradation Loss (VZBL) model. The VZBL model is a simpler analytical model that incorporates aerobic and anaerobic processes for prediction of hydrocarbon mass loss.

Results/Lessons Learned. A range of MIN3P-Dusty simulations are performed for a reference petroleum hydrocarbon composition. The relative importance of aerobic and anaerobic processes for hydrocarbon mass loss are quantified in the vadose zone and saturated zone for a range of LNAPL conditions. The influence of hydrocarbon component solubility and dissolution kinetics are shown to be potentially limiting factors resulting in slower degradation of heavier molecular weight alkanes. The results are qualitatively compared to available site data on hydrocarbon composition. The results of simulations considering the LNAPL distribution below the water table provide insight on site conditions where degassing based on pressures that are greater than hydrostatic could be significant.