Simulation of Variable Contaminant Decay in the Presence of a Decaying Carbon Substrate

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Background/Objectives. The selected remedy for groundwater impacted with hexavalent chromium was the injection of a carbon substrate to develop reducing conditions that would convert hexavalent chromium to the less mobile species of trivalent chromium. A site-specific numerical groundwater flow and solute transport model was developed (MODFLOW and MT3DMS, respectively), and a subsequent modeling analysis was conducted to determine the appropriate spacing, carbon substrate concentration, and dosing frequency for the proposed injection well network. MT3DMS was utilized to simulate fate and transport of both the carbon substrate and hexavalent chromium. As the injected carbon substrate is utilized by the microbial community and reducing conditions are developed, the injected carbon mass decays over time. As carbon injections were not intended to be continuous, MT3DMS was modified to only simulate the reduction of hexavalent chromium in the presence of carbon concentrations greater than a specified threshold carbon concentration. The threshold concentration is the estimated minimum carbon concentration that will continue to support reducing conditions.

Approach/Activities. The MT3DMS simulation code was modified (a two-species model for this application) to allow for the degradation of the first species (hexavalent chromium) only in grid cells where the second species (carbon substrate) exceeds a threshold concentration. Currently, the standard version of MT3DMS nor any publicly available modifications of the MT3DMS code exist that incorporate this modification. The modified version of MT3DMS was applied to the Site of concern, and the threshold carbon concentration was set to 0.01 mg/L. So, in areas where carbon concentrations were below 0.01 mg/L, the decay rate of hexavalent chromium was assigned a half-life of zero (0) days or no decay (i.e., background outside of the presence of carbon) while in areas where the carbon concentration exceeded 0.01 mg/L, the hexavalent chromium rapidly reduces to trivalent chromium under a half-life of one (1) day. The decay rate of the carbon substrate was assigned a half-life of 20 days based on injection pilot tests conducted at the Site. The threshold carbon concentration was estimated below typical carbon detection limits and the assumption of continued reducing conditions due to lysis effects. A series of sensitivity analyses were also conducted at various other carbon concentration thresholds to evaluate potential ranges in remedy operation.

Results/Lessons Learned. A modified version of MT3DMS that incorporated simulation of this carbon concentration threshold was applied to a relatively large hexavalent chromium plume using a well-calibrated site-specific numerical groundwater flow and solute transport model to help design an injection well network (spacing, dosing, and frequency) for an in situ remedy. The injection well network was designed to achieve reducing conditions across an entire transect of the hexavalent chromium plume, allowing for the ambient hydraulic gradient to transport the hexavalent chromium plume through the induced reducing conditions. The injection well spacing, injection rates, carbon concentrations, and dosing frequency were incrementally varied between model simulations until an optimal cost-effective remedy design was realized. The resulting design (developed with the model and modified transport code) was then implemented in the field. While local heterogeneities in the aquifer, which were not able to be accounted for in the model, resulted in some observed variations in injection rates, the injection system was primarily operated per the model-based design. Dramatic reductions in hexavalent chromium were observed as reducing conditions developed and the resultant clean water flush was produced across the carbon injection line.