Comparison of Three Mass Flux Estimation Methods Applied to a NAPL-Impacted Sedimentary Aquifer in Brazil

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Background/Objectives. An industrial site in Camaçari in the state of Bahia, Brazil, has been the subject of comprehensive site characterization efforts, both by traditional (e.g., soil and groundwater sampling) and high resolution techniques (e.g., MiHPT logging, borehole natural gamma profiling and Electrical Resistivity Imaging). Former site operations have resulted in a mixture of compounds being present in soil and groundwater; the primary compounds of Interest (COI) include chlorobenzenes, chloronitrobenzenes, BTEX and chloroanilines. To identify key zones where mass is transported and to support remedy decision-making, the data were used to calculate mass flux and mass discharge using three different methods, and the different approaches compared in terms of their strengths and limitations.

Approach/Activities. Mass flux and mass discharge were estimated using three methods:
1. *Direct transect method* based on concentrations measured in single-level monitoring wells, with hydraulic conductivity derived from slug tests and hydraulic gradients calculated for each well based on the potentiometric map. Mass flux and mass discharge were calculated for the four COI groups with ITRC´s Mass Flux Toolkit, along five curvilinear transects perpendicular to the groundwater flow direction and coincident with existing monitoring wells.
2. *Indirect transect method* with support of an Earth Volumetric Studio (EVS)-based digital model. 3-D plume shells were interpolated for the four COI groups. Hydraulic conductivity data were derived from pressure corrected high-resolution data of Hydraulic Profiling Tool (HPT) profiles, and grouped according to an updated hydrostratigraphic framework. A site-wide hydraulic gradient was used. Mass flux and mass discharge were calculated along the same five transects used in the direct transect method.
3. *Plume capture method* to calculate mass discharge based on data of an existing hydraulic barrier downgradient of the site, with pumping rates and concentration data derived directly from the pumping wells.

Results/Lessons Learned. The direct transect method allowed for identification of source zone hot spots and mass flux distribution, using data that were readily available and with minimal computational effort. The indirect transect method, based on the pressure corrected hydraulic conductivity data from the HPT profiles, allowed for the definition of preferential flow zones in the updated hydrostratigraphic framework, providing more useful information than the direct transect method. These first two methods have the limitation of uncertainties related to the sampling density and to interpolation errors. The plume capture method is unable to identify discrete high-flux zones, is highly sensitive to the applied pumping rates, and only allows for estimation of the total mass discharge rather than local mass flux distribution. However, the plume capture method is more likely to estimate the actual mass discharge across the capture zone of the pumping well(s) because this method intrinsically accounts for COI distribution and parallel variations in hydraulic conductivity.