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Estimating Quantities

The general topics of Estimating Average Concentrations, and Plume Change/Attenuation Over Time are related to Estimating Quantities (see General Topics, Table 2). Interpolated grids of contaminant concentrations created using simple geospatial methods can be used to quantify metrics such as average concentration, total mass, or volume of media above cleanup goals. Performing interpolations and calculating these metrics for sequential sampling events can be used to evaluate plume change over time (for example, shrinkage) visually or statistically by performing trend analysis on the metric in question.

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Manually calculating contaminant average concentration, total plume mass, or volume of media above cleanup goals or other criteria requires grid math or area/volume analysis tools in programs such as ArcGIS or Surfer. For example, average concentration can be calculated by dividing the integrated volume of the interpolated grid by its planar area (Ricker 2008). This procedure and a related procedure concerning calculation of plume mass are explained in detail in the example on plume shrinkage.

Another method is declustering using a grid or Voronoi polygons to determine weights to apply to spatially clustered data and use those weights when calculating average concentrations and total plume mass. This approach is similar to the MAROS automated calculations of plume mass. These operations can be performed for the entire extent of the data set or subset areas to evaluate whether concentration trends vary in different areas of a site. These operations can be performed on dissolved-phase concentrations (mass/volume of water) and soil concentration (mass/mass of soil) to better understand the total contaminant mass in the subsurface.

Regardless of the level of complexity of the selected method, the results from the geospatial analyses generally provide a better way to estimate mass and volume than simply averaging the results of individual data points and multiplying that value by assumed values of thickness or planar area. High or low concentrations may introduce bias into the model if the spatial extent of the measurements is not considered. This bias can be reduced by estimating values for unsampled locations using interpolation. The results can be used to optimize release detection and site characterization by highlighting areas with increasing average concentration or mass.

The results of these estimates can also support remedial design. For example, these results can be used to estimate how much of a remedial amendment (such as chemical oxidant or biological substrate) is necessary to treat the contaminant mass. Mass flux/discharge or mass reduction standards may be used as remedial goals, in which case these geospatial methods can be used to evaluate remedial success and optimize remedial efforts to focus on areas requiring additional mass removal. Additionally, visually and statistically demonstrating plume shrinkage in monitored natural attenuation (MNA) evaluations may be used to show that the remedy is effective and the site is progressing towards closure. Decreasing or stable plume conditions may be a prerequisite for site closure; these methods can therefore be helpful in demonstrating those conditions have been met (as with trend maps).

Using advanced methods such as kriging to estimate average concentrations and quantities and track plume changes may provide more defensible results because these methods incorporate spatial correlation of the data, as well as factors such as anisotropy. Advanced methods can also quantify the uncertainty of estimates, which may be critical when metrics such as contaminant mass are used for closure criteria. As with other uses of interpolation, consider site-specific features, which may influence estimates of contaminant mass and average concentrations. Also verify that the assumptions and results are consistent with the site CSM. This evaluation may include areas that were previously excavated and replaced with clean fill (from which no sample points may exist), or barriers to contaminant transport such as surface water features, bedrock outcrops, or faults.