White Paper

Development of Sediment Prisms in Lower Fox River OU1

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Abstract

This white paper describes the rationale and approach for use of a sediment modeling tool, GMS (Environmental Modeling Systems, Inc.), to delineate the lateral and vertical extent of PCB contaminated sediment deposits in Little Lake Butte des Morts (LLBdM), Lower Fox River, Wisconsin. LLBdM is commonly referred to as Operable Unit 1 (OU1) when described in the context of the Lower Fox River and Green Bay Record of Decision (ROD). Delineation of sediment deposits is an important component of the Remedial Design work in LLBdM.

GMS was used to organize sediment sampling data, to estimate the spatial distribution and volume of contiguous deposits with total PCB concentrations greater than the Remedial Action Limit (RAL), and to provide a platform for visualization and data export to CADD and other computer application environments. This white paper emphasizes the use of the GMS inverse distance weighted (IDW) approach in 3D (Shepard's method). The white paper also discusses the rationale for selection of GMS and the interpolation method, the general approach for use of GMS for 3D sediment modeling, and refinement measures used to assess and improve the quality of modeling results.

Ultimately, the primary goal for sediment deposit modeling is to accurately delineate regions of PCB contamination – so that remedial actions are successful in achieving remedial action objectives. Remedial designs need to address regions with total PCB concentrations above the RAL.

The economy and effectiveness of remedial designs depend on accurate delineation of the contaminated regions. The physical extent of the soft sediment deposits is used to establish an overall modeling boundary. PCB sample results are then used to interpolate contamination concentrations to a dense, 3D model mesh. The 3D mesh represents the PCB characterization of the deposit with high resolution. The specific modeling process with GMS for OU1 deposits is described in the white paper.

Typically, contaminated regions in OU1 are shallow, as data show contamination in only the top 12 inches (30 cm) over large areas. The stratified nature of sediment deposits can be incorporated within the IDW method, using a z-scale anisotropy factor. The IDW method considers nearest neighbor sampling points to the mesh, and weights the influence of each point inversely with distance. The z-scale anisotropy factor effectively stretches the distance in the vertical direction, so that points that are at the same depth at some horizontal spacing are given more influence. This weighting technique allows stratified deposits to be effectively modeled in 3D by considering possible correlations in the vertical dimension. This white paper discusses the rationale and implications regarding the selection of the z-scale anisotropy factor and the number of nearest neighbor points to consider for modeling work in OU1.

This white paper documents the current state of practice for sediment modeling in support of the remedial design for OU1.

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1. Introduction

This white paper has been prepared in response to a request by the Wisconsin Department of Natural Resources (WDNR) to present the methodology used to identify boundaries of polychlorinated biphenyl (PCB) contaminated sediments in Lower Fox River Operable Unit 1 (OU1).

1.1   Purpose and Scope

The purpose of this white paper is expressed in three parts:

1) address the rationale for development of PCB contaminated sediment prisms in OU1 using three-dimensional modeling software;

2) describe the three-dimensional (3D) modeling approach and associated software (GMS[1]), and;

3) discuss refinements applied to GMS for the application of modeling contaminated sediment deposits in OU1.

Following this introductory section, Section 2 describes the general modeling approach and Section 3 presents the measures that have been taken to refine the GMS model for use in OU1. Although GMS is intended for a wide range of geo-environmental applications (GMS, 2002), the scope of this white paper is limited to application of GMS for modeling PCB contaminated sediment deposits in OU1.

1.2   Background

The specific goals and strategies employed to date for site characterization and sediment modeling in OU1 have varied for the Fox River Mass Balance Study, the Remedial Investigation (RI), the Feasibility Study (FS), and the Record of Decision (ROD). This white paper addresses how 3D sediment modeling meets the needs of the remedial design/remedial action phase of the project. Additional background on the RI/FS methods and ROD requirements are also provided.

1.2.1   RI/FS Methodology

The goals of deposit modeling methods used for the RI/FS were to provide estimates of PCB mass distribution and the potential impacts of contaminated sediments, as well to provide estimates of sediment volume and sediment properties needed to evaluate remedial options.

Historically, WDNR has employed a two-dimensional (2D) interpolation modeling strategy in OU1 to estimate sediment volumes, sediment thicknesses, and PCB mass associated with particular deposits. WDNR's model evaluated PCB contamination in sediments using independent, multiple layers of sediment sorted by increasing depths – and incorporated a 2D interpolation method with the following attributes:

- ♦ Inverse distance weighting (IDW) with a power parameter of 5.

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[1] GMS is a computer application licensed by Environmental Modeling Systems, Inc., South Jordan, Utah.

♦ Interpolation radius of 400m (1230 ft.), with data segregation in 10 m square grids, and depth intervals of 0-10 cm, 10-30 cm, 30-50 cm, 50-100 cm, 100-150 cm, 150-200 cm, 200-250 cm, 250-300 cm and >300 cm.

A more detailed description of the interpolation method used by WNDR is presented in the Final Model Documentation Report (WDNR, 2002a).

1.2.2 Record of Decision Requirements

The ROD for OU1 and OU2 was issued by WDNR and U.S. EPA in December 2002 (WDNR, 2002b). For OU1, the ROD requires that pre-design sampling and characterization work define the horizontal and vertical extent ("footprint") of the sediment with a total PCB concentration above the Remedial Action Limit (RAL) of 1 ppm. A portion of this footprint will be dredged while other portions could be amenable to capping as the contingent remedy.

The ROD did not specify a method or model that should be used to estimate the RAL footprint.

1.2.3 Use of Model for Remedial Design

In August 2003, a pre-design sediment characterization report for Deposit A presented an approach for delineating the RAL footprint (Foth & Van Dyke, 2003). The model in the characterization report uses a three-dimensional (3D), inverse-distance weighted (IDW) interpolation method and the computer application GMS version 4.0.

GMS has since been used for more detailed modeling work in OU1 to support engineering evaluations, project planning, and the remedial design. While the WDNR 2D model was suitable for the RI/FS, the GMS-based, 3D model is considered to be more applicable and useful to the design process where 3D grading plans for setting of dredge grades and more precise volume determinations are required. Since the model varies from the WDNR model, this white paper was generated to more fully discuss the rationale and methods for the 3D modeling process.

For deposits that are to be dredged or capped, the economy and effectiveness of remedial designs depend largely on accurate delineation of the contaminated regions. Doing this well is a technical challenge with high stakes, and two major tradeoffs. The first tradeoff is one of sampling density. Accurate delineation of contaminated regions generally increases with greater sampling density, but sampling and analysis costs also rise accordingly. Effective sample designs often use modeling tools, adaptive sampling techniques and staged approaches to optimize the sampling plans. The second tradeoff deals with the level of conservatism used to address uncertainty in the remedial design. If there is a relatively uncertain delineation of the contaminated region, the certainty of removal of contaminated regions generally increases as more sediment is removed. However, remediation costs are directly related to the amount of sediment to be removed and processed. Poor delineation and excessive removal of cleaner sediment can have large cost consequences.

Deposit modeling for accurate delineation of contaminated regions provides a critical link between sampling and remedial actions. The extent of the soft sediment deposits is used to establish a modeling boundary, and sample results are used to interpolate contamination

concentrations to a dense, 3D model mesh. The 3D mesh then represents the characterization of the whole deposit with high resolution.

1.3 Rationale for Selection of GMS and IDW Methods for Sediment Modeling

The rationale and criteria for the selection of GMS and the IDW method for sediment modeling in OU1 are discussed below

1.3.1 Need for Model to Match Characteristics of Sediment Deposits

There are several general aspects of Lower Fox River OU1 sediment deposits that are important in the selection of a modeling tool:

- Soft sediment in the river is composed of silts and silty clays, and most of the PCB contamination is found in the soft sediments.

- Soft sediment thickness generally ranges from 0 – 6.5 ft. Soft sediment deposits may be bounded laterally by shoreline or by fine sand and gravel deposits. Near these boundaries, soft sediment thickness may be negligible. With depth, soft sediment is most often bounded by a clayey, glacial till.

- Soft sediment thickness may vary by 0.5 ft. or more in distances of 100 ft. or less.

A large portion of the PCB mass found in OU1 soft sediment deposits has been found in the upper 1 foot (30 cm) of sediment. For example, WDNR estimated that Sub-areas A, E, and POG contain about 91% of the PCB mass present in OU1. For these sub-areas, about 53% of the PCB mass is present in the upper 1 foot (30 cm) of sediment (WDNR, 2002c.).

Sub-area A data indicate a relatively shallow zone of PCB contamination over an area of roughly 40 acres. While WDNR estimates 53% of the PCB mass of certain deposits is located in the top 1 ft., it is also relevant to the design aspects of the project that 88% of the samples reporting above the RAL were found in the top 1 ft (WDNR 2002c).

Modeling to support delineation of PCB contaminated sediments in OU1 should, therefore, be scrutinized with respect to accuracy with depth. Suitable models should "capture" contaminated samples at depth without establishing dredge prism elevations that would result in excessive removal of sediments with PDB levels less than the RAL.

1.3.2 Need for 3D Interpolation of Sediment Deposits

Contaminated sediment deposits tend to be stratified vertically. Previous attempts to estimate contaminated sediment deposit volumes have been based on a 2D interpolation method (WDNR, 2002a). This method effectively treats the deposit as if there was no correlation of PCB concentration occurring in different sediment layers. 2D interpolation is also made more difficult if the sampling interval with depth is irregular, if datasets from different sampling periods are combined, and if the deposit includes channels, eddy features, or sand ridges.

A 3D interpolation strategy can offer a more refined characterization of the sediment deposit concentration trends and the deposit volume. An idealized profile of a soft sediment deposit is

shown in Figure 1.1. By considering the potential correlation of sediments at various sediment depths, 3D interpolation offers a more accurate representation of the sediment deposit. In addition, the ease of use is increased because less preprocessing of data is needed to assign a given sample to a model layer.

Since the correlation of PCB concentrations with depth is generally much less than with lateral distance, 3D interpolation methods that account for vertical heterogeneity are more appealing. For instance, in certain shallow deposits, contaminant concentrations at different positions may be completely uncorrelated at vertical distances of 2 ft., as compared to lateral distances of 300 ft. However, at greater depths, the degree of horizontal correlation in PCB concentrations may be much less. 3D interpolation offers flexibility in selecting modeling parameters to provide an acceptable match to the data horizontal and vertical distribution. There is a balance that can be reached between the accuracy of concentrations predicted at the surface versus effective delineation of the contamination at depth. As normally applied, 2D interpolation lacks this general flexibility offered by 3D interpolation models.
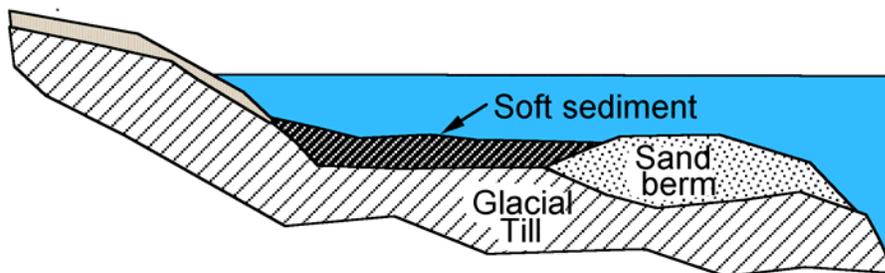
Figure 1.1   Idealized Profile of Soft Sediment Deposit Where 2D Interpolation May Fail to Accurately Delineate the Deposit.

1.3.3   Selection of GMS as 3D Interpolation Tool

GMS (v. 4.0, Environmental Modeling Systems) is one of several available platforms to perform 3D interpolation. GMS provides powerful tools for digital terrain modeling. In fact, GMS is organized around a set of terrain modeling tools that were first developed for cut-and-fill imaging and volume calculations used in civil and geotechnical engineering (Jones 1990, Jones and Wright, 1993). Research and development of the terrain modeling tools at the University of Texas at Austin was supported by the US Army Corps of Engineers. Further development of GMS (Department of Defense Groundwater Modeling System) was led by Prof. Norm Jones and Jim Nelson of Brigham Young University, with funding from the U.S. Department of Defense, the Department of Energy, the Environmental Protection Agency, and the Environmental Modeling Research Laboratory at Brigham Young University.

GMS offers the use of several 3D interpolation methods, including kriging, natural neighbor, and various IDW methods. Other factors that led to the selection of GMS for estimating contaminated sediment deposit volumes were:

1. Accuracy. Prior to commencing dredging activities the stakeholders should be confident that, by following the dredge plan, effective removal to the RAL will occur. The interpolation options and basic methods within GMS have been tested and verified

for accuracy as described in Section 2 of this white paper. In addition, the flexibility of modeling options allows for ongoing refinement to improve the quality of the estimates.

2. Capture of sample points with total PCB concentrations above the RAL. GMS can be used with other graphics and analysis packages to verify that all sample points with concentrations above the RAL are included in the RAL isopach. While it is possible that the interpolation methods employed may not capture isolated samples with concentrations above the RAL, supplemental data processing strategies are used to identify outliers. Once identified, outliers can be incorporated into the overall dredge scheme if appropriate.

3. Use of GMS as a sampling design tool. GMS may be used to identify regions of sparse sampling near the PCB isopach boundary. As such, GMS is useful as a sampling design tool for future sampling efforts (if needed) to refine the isopach delineation.

4. Validation. Ability to test statistical properties of interpolated results, jackknife interpolation, and other geostatistical methods.

5. Compatibility with CADD. Mapping data can be imported into GMS from CADD (or equivalent program), and results of surface models and interpolated PCB isopachs at the RAL from GMS can be exported to CADD (or equivalent program). GMS also offers compatibility with spreadsheet and plotting applications.

6. Ease of use, ability of others to review results. A demonstration version of GMS is available for the public, offering reviewers an opportunity to review datasets and methods used in GMS. GMS is widely distributed at the U.S. Army Corps of Engineers, and is available to US EPA and other federal agencies.

7. Visualization. GMS offers outstanding visualization features, including color contours, shaded surfaces, cross-sections, and animation. Graphics can be exported to image files for display and presentation.

Although GMS has a wide range of features, other applications with overlapping features may be used. In particular, CADD (or equivalent program) is used to provide higher-resolution maps, to prepare engineering drawings such as dredge grading plans and cross-sections, as well as output files for use by dredging contractors (e.g., DXF or DGN files for Dredgepack® software[2]).

1.3.4 Selection of GMS Interpolation Algorithms

Several interpolation algorithms are available within GMS. GMS work to date on OU1 has been based, almost exclusively, on the use of a modified inverse distance weighted (IDW) method. This method is also called Shepard's method because the power (p) of the weighting function is 2 (Shepard, 1968). GMS implementation of the Shepard's IDW method uses a normalized weighting function (Franke & Nelson, 1980) that differs somewhat from the classical IDW weighting function.

Factors which have led to a preference for the use of Shepard's IDW method in 3D over other alternatives (kriging, other IDW methods, natural neighbor, and others) include:

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[2] Dredgepack® is a registered computer application from Coastal Oceanographics, Inc., Middlefield, CT.

1. WDNR used a 2D IDW method in order to develop sediment volume and PCB mass estimates for the Lower Fox River RI/FS studies.

2. Suitable agreement to sampling data were found with Shepard's method. The kriging algorithm in GMS, even after multiple trials, was not found to produce results in 3D that were representative of the sampling data.

3. A particular advantage of Shepard's method is its ability to address vertical heterogeneity. In addition, Shepard's method works relatively well in subregions of low sample density as well as high sample density.

Limited evaluations of natural neighbor and other IDW algorithms within GMS have been considered unsuccessful, because of poor overall model performance (inaccurate predictions, slow processing time, and memory-related application errors). These limitations have generally not been found when using Shepard's method.

While Shepard's method will likely continue to be the preferred interpolation algorithm for OU1 deposits, other algorithms could prove to be more representative for some deposits given deposit-specific sampling schemes, data sets, and geometry.

1.3.5   Current State of Review of GMS

GMS has been applied and discussed within a previous Sub-area A sediment characterization report (Foth & Van Dyke, 2003). Since then, GMS has been used to refine estimates in other OU1 sediment sub-areas. To date, GMS has been used for Lower Fox River deposits to:

- organize and display sediment core sampling data,
- model the geometry of certain deposits (shoreline boundary, top of sediment, soft sediment thickness),
- estimate the volume of sediment and sediment properties above a threshold or limit concentration, and to
- visualize spatial trends in contaminant concentration.

This white paper addresses the current state of GMS as applied to OU1.

2. GMS Approach for OU1

This section summarizes the general approach for the use of GMS to model contaminated sediment deposits in OU1. This section addresses the main steps used to:

- enter sediment sampling data into GMS
- form the sediment deposit mesh
- perform the interpolation
- calculate the isosurface volumes
- export the results to CADD (or equivalent program)
- visualize the results

2.1 Entering Sediment Sampling Data

For Sub-area A, the general strategy for composing the active dataset for GMS is to initially include all the validated 2003 Pre-design sampling data and data from the WDNR Fox River Database (FRDB), then to edit points according to an explicit process and usage criteria. These criteria are discussed below. The active data sets for other sub-areas are initially constructed with 2003 Pre-Design sampling data alone, and may be enhanced with Phase 2 sampling data and/or historical data from the FRDB if data gaps are evident.

Sediment sampling data can be loaded into GMS from simple, delimited text files. The text import routine supports a variety of formats and data type targets. In this case, sample data are loaded as 3D scatter point sets. A sample data file format is shown in Table 2.1. The elevation coordinate (Z) is loaded in units of feet, as the elevation relative to the top-of-sediment (e.g., if the sample was at a depth of 1.3 ft., the value of Z would be listed as –1.3). [3]

Core sample data are reported for a sampling interval, but GMS treats each sample as a point value. As a representative value for PCB interpolation, the elevation at the middle of the sample interval has been used. .

Table 2.1 General Format for Sediment Sampling Data to be Loaded Into GMS.

Sample I.D.	X (ft.)	Y (ft.)	Z (ft.)	PCB (ppm)	Percent Solids	TOC (ppm)
C-01-A	2369210.02	806441.23	-0.33	6.0	16	-999
C-01-A-C	2369210.02	806441.23	-0.66	2.3	24	-999
C-01-D	2369210.02	806441.23	-0.98	0.089	27	-999
C-01-E	2369210.02	806441.23	-1.31	0.064	27	-999
C-02-A	2369325.41	807046.64	-0.33	0.049	53	-999

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[3] WDNR's preferred vertical datum for the Lower Fox River sediment remediation projects, as of July 2003, is NAVD 88, and the horizontal datum, WTM 83. Final Design outputs for dredge elevations and post dredge verification work will conform to these datums.

Total PCB concentrations are loaded in units of mg/kg (ppm). If the reported PCB concentration is less than one-half of the reported detection limit (RDL) for that sample, the PCB concentration is assigned the value of one-half the RDL. Percent solids (%),TOC (mg/kg), and other data may also be entered. Missing values are assigned a missing value flag (commonly –999).

2.1.1   Interpolation Set Data Exclusion and Addition Criteria

In general, the exclusion of real samples and inclusion/modification of data values at specified locations is avoided – so that geostatistical properties of the dataset are properly reported as input to the model. In addition, a record for all OU1 sampling data is kept in a multiple worksheet spreadsheet file (MS Excel or other spreadsheet application), listing the data considered, the data used for GMS, added data points, and the data excluded. Sample data used for each sub-area model are also clearly described.

There are limited cases for which sample data are excluded and other values are added to the active GMS dataset. The criteria and rationale for editing data values in the active GMS set are listed below.

Criterion #1:   Exclude duplicates.

Rationale: Since GMS cannot load multiple 3D scatter point data at the same point in space, duplicates are removed prior to loading the set into GMS.

It is important to note that duplicates are clearly marked prior to analysis and that duplicates were obtained for analytical QA/QC purposes only. Exclusion of duplicates was based on sample identification prior to delivery to the laboratory, not the lab-determined concentrations of the primary or duplicate samples.

Criterion #2:   Exclude sample data from full-length composite core samples, unless the sampling depth is shallow, there are no other sampling locations nearby, or if the PCB concentration is below the RAL. The criterion applies to historical (pre-2003) data only.

Rationale: In certain datasets for Sub-area A, some samples were collected from composite samples incorporating the entire core length, with a resulting thick sampling interval from the surface to depths of 3 ft. or greater. However, nearly all recent samples (2002 and newer) are more consistently collected and analyzed with relatively thin sample intervals (e.g., 0 – 10 cm or 0 – 0.33 ft.). Since the majority of PCB contamination is present in the upper 1 foot of OU1 Fox River sediments, it is likely that the process of including data from a full-length composite core sample would lead to an inaccurate assessment of PCB contamination at depth. For example, where a core with many samples may show high PCB concentrations to a depth of 1.0 ft. (but low PCB concentrations from depths of 1-3 ft.), a 3-foot composite core sample collected at the same location could be misinterpreted as a sample with high PCB concentration to it's mid-point depth. Alternatively, if a historic composite core sample reports a PCB concentration below the RAL, it is appropriate to include the sample since the sample is expected to have a PCB concentration near or below the RAL over the whole depth.

Criterion #3:   Represent sample stations with "no soft sediment" as a surface sample.

Rationale: WDNR allows special consideration of sampling stations if no sample could be obtained due to the physical absence of soft sediment. In such cases, we have assumed the PCB concentration at the sampling location to be 0.025 ppm, the average PCB concentration determined from 7 samples taken below soft sediment at the top of the native clay layer in Sub-area A during the Foth & Van Dyke 2002 sampling event (Foth & Van Dyke, 2003). The sample ID is designated by the name of the sampling station and the suffix "–NS". For example, no soft sediment was found at Sub-area A sampling station A13, so the sample point is named "A-13-NS" and assigned a depth interval of 0.00 – 0.10 ft. For all of OU1, there were 116 stations at which –NS designations were assigned and added to the active GMS sample dataset which totals approximately 5100 samples.

Criterion #4:   Exclude older samples at locations for which more recent confirmation sampling is applied at the same, or adjacent location.

Rationale: Confirmation sampling is a tool to determine whether or not a former sample was correctly quantified, or whether or not conditions have changed at a particular sample location. For the cases in which additional, more recent sampling is specifically targeted to address uncertainty at the same location as a prior sample, the more recent sample is retained and the prior sample is excluded. A comment is added to the excluded sample record, indicating that it was replaced by a confirmation sample. For the active GMS dataset for OU1, samples taken in 2000 at station LLBM-A-80 were excluded (FR1279 and FR1280, PCB concentrations 2.06 ppm and 0.08 ppm, respectively). Confirmation samples (with the same sample intervals) collected at station A-28 in 2003 (A-28-A, A-28-A-C) revealed lower PCB levels (0.41 ppm, 0.04 ppm respectively) at this location at the same depth intervals.

2.2   Developing Surfaces for Upper and Lower Extent of Sediment Deposit

Modeling of the sediment deposit as a continuous 3D solid requires generating surfaces to describe the top and bottom of the sediment, and using GMS tools to build 3D meshes, 3D grid models, or other solid object representations. Surfaces are described by triangulated irregular networks (or TINs). TIN nodes can be imported as 2D scatter point files, or created within GMS. The TIN nodes are points with 3D position coordinates (XYZ). GMS uses automatic triangulation algorithms to connect the nodes into a network of triangles. Upon triangulation, the TIN nodes become the common vertices of the triangles.

2.2.1   Setting Horizontal Extent of TINs

TINs are confined by the shoreline, and, if desired, any predetermined sub-area boundaries. In general, the TIN should extend beyond all sampling locations in the deposit – or, at least, all sampling points in the deposit with PCB concentrations near the RAL. It is important to note that sample subsets from adjacent sub-areas may be included in the interpolation, even though these points lie outside the modeled sub-area boundary.

 Boundaries should be imported to GMS from CADD (or equivalent program) to define the shorelines and sub-area boundaries. It is important that CADD and GMS boundaries and other mapping objects be accurately positioned and consistent.

2.2.2 Setting the Horizontal Resolution of the TINs

Setting the horizontal resolution, or the TIN density, is a decision made by the modeler based on site-specific conditions. In general, TIN density should be considerably higher than the sampling density, be set to allow effective delineation of the shoreline and other boundaries, and be limited to a manageable total number of TIN vertices.

For Sub-area A and other OU1 sub-areas with a more uniform sample grid spacing (e.g. 230' or 350' triangular), the TIN density is established using a uniform 30 ft. triangular grid with the inclusion of actual sample locations as additional TIN nodes. The characteristics of surface TINs for Sub-areas A and C are summarized in Table 2.2. A preliminary image of the top TIN surface for Sub-area C is shown on Figure 2.1.

Table 2.2   Characteristics of Surface TINs Used to Describe OU1 Sub-areas

Sub-area	TIN vertices	TIN triangles	TIN area (Ac)	Average number of TIN nodes per acre	Average number of triangles per acre	Average number of sampling stations per acre
A	4231	8189	71.4	59	115	2.0
C	1158	2128	18.6	62	115	1.0

Figure 2.1 Preliminary Surface TIN for Sub-area C. Positions of sampling stations (•) and grid lines spaced at 500 ft. (---) are also shown.

2.2.3   Developing the Top TIN

The upper surface, or top TIN, may be flat or contoured to portray the top of sediment. Experience to date with GMS has shown that the flat TIN top surface works best, for two reasons. The first reason is that the interpolation results were found to be more representative with a flat model. Although efforts have been made with OU1 data to use an elevation-based top TIN, the resulting volume estimates have been larger than physically possible (given the deposit area and average soft sediment thickness). The errors that occur are likely due to an implied correlation of PCB concentrations with elevation (rather than depth). Performing the same operations with a flat top TIN produces a more reasonable volume estimate. The second reason is

that most of the WDNR archival sampling data are reported in terms of sample interval depths (not elevations). Building an elevation-based top TIN would require the estimation of the elevations for these sets. Converting the depth-based isopachs to elevation-based maps for design plans is easily accomplished using elevation-based surface data collected during the 2002 and 2003 OU1 sampling events.

2.2.4   Developing the Bottom TIN

The lower extent of the interpolation region, or bottom TIN, is designed to be contoured to match depths to a confining layer. Since the bottom TIN will define the lowest extent of the 3D mesh, the design of the bottom TIN can be a crucial step towards the goal of accurate delineation of contamination in a sediment deposit. The following guidance is offered:

♦ Evaluate core logs and sediment probing data to determine the thickness of the soft sediment in the sub-area.

♦ Evaluate the sample data to determine the lowest extent of PCB contamination above a threshold value. The depth of the bottom TIN should extend to a depth greater than the lowest sample with a PCB concentration over a threshold value (i.e., a RAL).

Once the mesh is formed and PCB sampling data are interpolated to the mesh, there may be additional modeling steps to accurately delineate the lower extent of contamination. These steps should include:

♦ Comparison of isopach depth versus mesh extent. If there is evidence of deeper contamination in soft sediment beneath the bottom TIN, the bottom TIN would need to be extended to greater depth.

♦ Evaluation of samples below the bottom TIN. If a given sample has a PCB concentration above the RAL, and is beneath the bottom TIN, the bottom TIN would be extended to provide "capture" of the sample point.

2.3   Developing the 3D Mesh for Sediment Sub-area Calculations

A 3D mesh is used as the primary 3D solid model of the sediment deposits. A 3D mesh is a connected network of multiple, triangulated layers. 3D scatter point data, such as PCB concentrations can be interpolated to the nodes of the 3D mesh. Data values produced from interpolation, such as PCB concentrations or percent solids values, are stored at each mesh node. Imaging and volume calculation tools can then be used to explore and reveal properties of the sub-area.

Once the top and bottom TINs are formed, 2D and 3D meshes can be generated. The 2D mesh can be formed directly from the top TIN. For this process to work smoothly, the 2D mesh, top TIN, and bottom TIN need to be aligned with the same XY coordinates and have the same number of nodes. The 3D mesh requires the existence of a 2D mesh, and is formed by selecting the top and bottom TINs, then "filling" between the TINs with a number of uniformly spaced layers. The maximum vertical spacing can be set to the smallest depth interval for sampling (such as a 4 in. or 10 cm spacing).

2.4   3D Interpolation to the Mesh

For OU1 sediment sub-areas the GMS implementation of Shepard's method has been used almost exclusively for interpolation of PCB sample concentrations to the 3D mesh. The interpolation routine requires the selection of two main parameters, the number of points used in calculating interpolation weights (N_p) and the z-scale anisotropy factor (α_z). If $N_p = 10$, the interpolation algorithm considers the 10 nearest points to a mesh node, calculates the interpolation weights based on distances, and uses these interpolation weights along with the concentrations at the nearest 10 sample points to determine the PCB concentration at the mesh node. The interpolation weights are larger for smaller distances between the sample point and the mesh node.

The z-scale factor, α_z, is a model parameter to compensate for the anisotropy in the vertical direction. If the distances between scatter points along the vertical traces are significantly smaller than the differences between scatter points along the horizontal plane, the effects of clustering along vertical traces can be minimized using the z-scale factor. For instance, if a z-scale factor of 100 is applied, a vertical distance of 1 ft. would be treated with the same weight as a horizontal distance of 100 ft. This can result in improved accuracy, especially for cases in which the degree of horizontal correlation is significantly greater than the vertical correlation, as is the case with OU1 sediments.

One strategy for setting IDW parameters is to select a z-scale factor from the ratio of horizontal and vertical sample spacings. For many sub-areas in OU1, the horizontal spacing is roughly 250 ft. and is based on an even triangular grid. The common vertical spacing is 4 in. (0.333 ft.). A z-scale factor set to the ratio of horizontal to vertical sample spacings, therefore, would be 750.

Initial selection of α_z and N_p can also be based on jack-knife interpolation results. One data point is temporarily excluded, and the rest of the set is used to interpolate a data value at that isolated location. This is done for the whole set, and errors between the interpolated values and the actual dataset are summarized. Once selected, the interpolated parameters should be optimized, if necessary, to maximize capture of sample locations with PCB concentrations exceeding the RAL, and to minimize excessive dredging at locations known to contain PCB concentrations below the RAL, as described below.

The main objectives are to maximize capture of all locations with PCB concentrations above the RAL and to minimize excessive dredging at locations known to have PCB concentrations below the RAL. The evaluation of jack-knife errors, therefore, will be most effective when there is particular focus on the quality of PCB concentration estimates for sample points that are expected to be located near the RAL isopach. Evaluation of jack-knife errors without this focus can be misleading, since the errors at a few points, particularly at sample points with the highest concentrations, can overwhelm the errors that may be more useful for delineating PCB concentrations near the RAL.

For most sub-areas in OU1, we have found excellent capture with a range of z-factors when the interpolation neighborhood is relatively small ($N_p = 4$ or $N_p = 8$). However, in order to also minimize excessive dredge cuts (with depth or horizontal extent) into regions with sample concentrations below the RAL, the z-factor is adjusted.

Once these two interpolation parameters are set and the 3D PCB scatter point dataset is selected, the user applies the command to interpolate that set to the 3D mesh. The 3D interpolation assigns PCB concentrations to all nodes of the mesh. Relatively dense meshes may have 50,000 node points or more. Mesh post-processing options within GMS include volume calculations, visualization and statistical tools to evaluate the data distributions.

2.5   Isosurface Volume Calculation

An isosurface is the 3D equivalent of the contour line. Each isosurface represents a certain concentration level. GMS uses interpolation between 3D mesh nodes to estimate the location of the isosurfaces. As the volume representing the subregion with a total PCB concentration above the RAL is of the most interest, the discussion below will focus on the RAL isosurface.

Since subregions with total PCB concentrations above the RAL may be clustered and discontinuous, the RAL isosurface may actually be a set of isosurfaces. There are a few aspects of isosurfaces that are particularly relevant to the estimation of sediment volumes. These aspects are:

♦ A higher mesh density generally provides for more precisely located isosurfaces. Since linear interpolation is used to estimate the location of an isosurface (between mesh nodes), the user may be assured that the selected interpolation method is responsible for the location of an isosurface when there is a higher density mesh. In addition, the curvature of an isosurface is better estimated with a higher mesh density.

♦ The generated isosurface may have an irregular shape and may extend the full depth of the mesh. A depth profile of an isosurface, such as is shown on Figure 2.2, may show isolated clusters of cleaner sediment, with PCB concentrations below the RAL, embedded within the RAL isosurface region. The region to remove (dredge) should extend from the top of sediment to the deepest extent of the isosurface – and this removal region could be described as a TIN or an isopach

♦ The isosurface may not capture all sample scatter points with PCB concentrations above the RAL. This is possible when an isolated sample point is slightly above the RAL, and other concentrations in the same area are well below the RAL. If the interpolated concentration at the nearest mesh nodes is below the RAL, a RAL isosurface will not be developed near the isolated sample point. This effect can be reduced if the mesh nodes are aligned to the sample points.

♦ The RAL isosurface may extend into subregions in which no sample has a PCB concentration above the RAL. This is possible when a subregion of highly contaminated material is adjacent to a relatively clean area. The influence of the samples with higher concentration may be greater than the influence of samples with lower concentrations that happen to be closer to the mesh nodes.

♦ The RAL isosurface may extend into subregions in which no samples are present. For this reason, it may be necessary to provide additional sample points to further delineate the RAL isosurface (Phase 2 sampling). With depth, it may be important to consider whether the RAL isosurface has extended into a confining glacial till or rock unit.

Alternatively, the deepest extent of the mesh could be confined to the regions of soft sediment (see sections 2.2.4 and 3.2.1 for further discussion).

Isosurface volumes can be verified by CADD (or equivalent program) and by other external calculation methods. Exported data for the RAL isosurface is used to develop a RAL isopach surface for CADD (or equivalent program). One simple check to evaluate the validity of the magnitude of the interpolated isosurface volume is to estimate the mean depth of the isosurface, then to multiply that estimate by the surface area of the isosurface.

Once the PCB-contaminated sediment delineation at the RAL has been interpolated using GMS, and the isosurfaces exported to CADD (or equivalent program), the sediment removal plans (dredge grading plans) will be engineered taking into account dredging accuracy, allowable overcut, and appropriate side slopes. Therefore, the implementation dredge prism volumes will likely exceed the GMS interpolated volumes at the RAL in each sub-area.
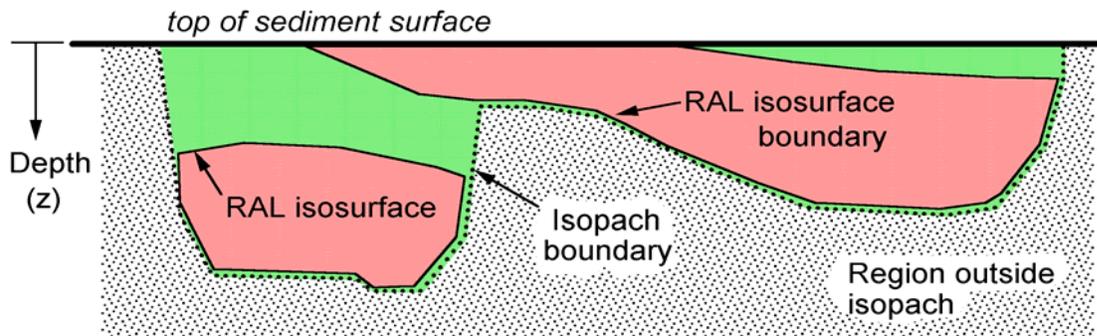

Figure 2.2   Idealized Depth Profile Used to Distinguish Removal Prism (Isopach) From Isosurfaces at a Set RAL. Isosurfaces are the result of interpolation and delineate regions with PCB concentrations above the RAL (shaded light red). Removal prism (isopach) extends from the top-of-sediment surface to depth to include all RAL isosurfaces and some cleaner regions (shaded green).

2.6   Visualization

GMS can be used to generate color images, sections, and video streams to better visualize sediment deposit characteristics. Once the 3D mesh is generated and data values are interpolated to the mesh, there are a wide variety of visualization features available to the user. These include:

- plan view, profile views, oblique (isometric) views from any compound angle,
- contour plots,
- shaded surface plots,
- sections and
- animation (.avi file generation)

Interpolation results can be compared visually to color-coded sample scatter points. Cut away sections can be used to isolate specific exposures of the sediment deposit. An example cardhouse section image for a sediment deposit is shown in Figure 2.3.
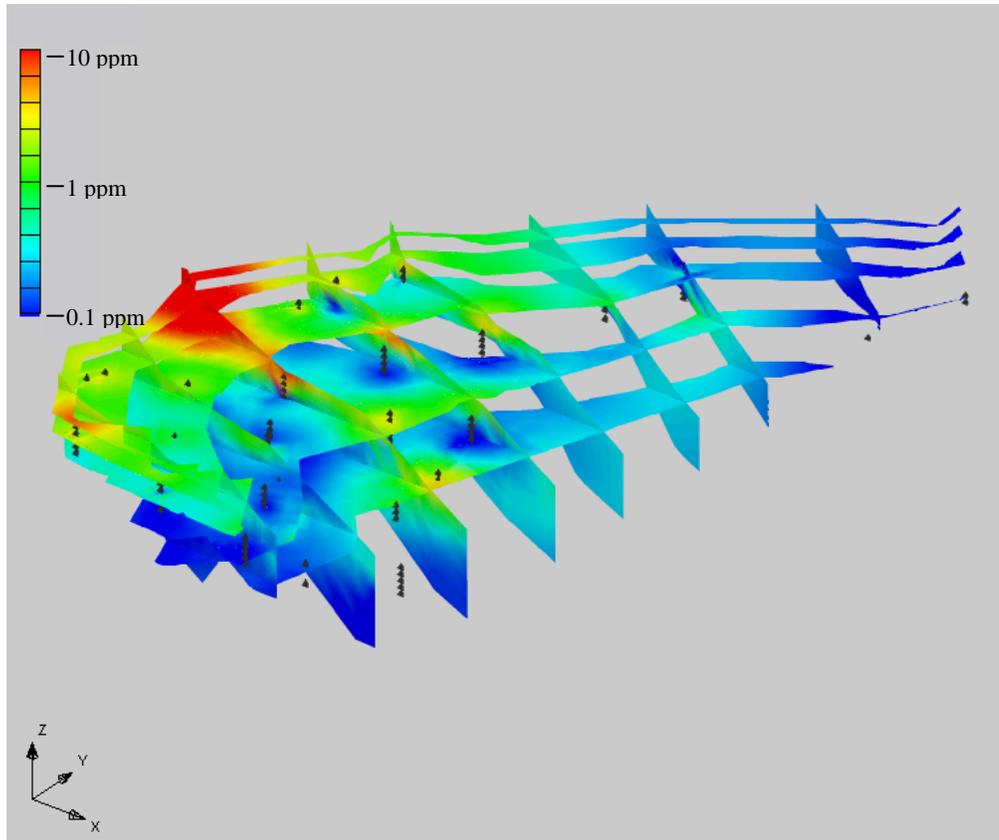
Figure 2.3   Cardhouse Representation of PCB Concentrations in a Sediment Deposit. Vertical scale is exaggerated 100 times.

2.7   Export and Ease of Review

GMS supports several common file formats for data export. GMS offers coordinate conversion and other tools to coordinate mapping and image data. In addition, a full function demo version of GMS (saving, export features, and printing disabled) is available for reviewers (see http://www.ems-i.com/gms for more details).

Supported export formats for GMS include:

- text file export of 3D mesh data (node id, X, Y, Z, data values)
- text file export of TIN data
- text file and .dxf export of map data
- image file export (.tiff)
- other formats

Data are easily copied-and-pasted into spreadsheet applications. Import and export of scatter-point and DXF image data between GMS and CADD are straight-forward.

3. Quality Assurance and Model Refinement

This section addresses several quality assurance and model refinements methods used to aid the characterization and analysis of sediment deposits.

3.1 Testing "Capture" of Scatter Point Sets

Since there are often many sampling data points with a range of PCB concentrations, it is sometimes difficult to review the sampling scatter points graphically in GMS. As such, other graphics applications can be applied in which a data filter strategy is utilized. Plan view plots of the sub-areas are viewed with the following criteria for the scatter points:

- Show only sample points above a threshold PCB concentration (at RAL)
- Show only sample points below a given depth (0, 1, 2 ft.)
- Color the plot symbol relative to PCB concentration

Using this plotting strategy, one can quickly identify the general distribution of samples at various depths that exceed the RAL and compare these observations with GMS views of the interpolated isosurface, or superimposed plots of the 3D mesh.

3.2 Model Refinements to Improve Model Outcomes

There are several refinements that may be used within GMS to improve model outcomes. These include ways of identifying and correcting inaccurate isosurface volumes, discarding sample data outliers, and using data truncation as an interpolation option.

3.2.1 Inaccuracy of Isosurface Volume

As a check, GMS provides the results of the calculation of mesh volume with the reporting of the isosurface volume. If the error is appreciable, isosurface volume estimates are scrutinized. Efforts to reduce the errors may include applying slightly different interpolation options, expanding or refining the mesh, or checking the volumes of isosurfaces that may correspond to different concentration levels.

As described in Section 2.5, isosurface volumes are checked by CADD (or equivalent program) and other external calculation methods. A large relative error may indicate a problem with the interpolation routine.

3.2.2 Discarding Data Outliers

As an example, for work in Sub-area A, an evaluation of the historic data from the FRDB resulted in a decision to exclude some of the older data from the GMS interpolations. The samples that were excluded were from full-length composite cores collected over sample intervals as large as 70 cm. Since the middle depth of the sample interval is input as the sample depth (z) in our GMS interpolations, a large inconsistency is found when comparing these samples with more recent, nearby samples with thin sample intervals.

For samples that were from the composite cores, the PCB concentrations were more reflective of

the more recent samples collected near the surface. Nearby samples with intermediate depth intervals below 1 ft. were typically found to have low or nondetect PCB concentrations. Therefore, there was strong justification for excluding the few samples from composite cores from the interpolation dataset.

3.2.3   Truncation

An option within the interpolation methods is truncation. Interpolation data can be truncated to fit within the range of existing data (controls extrapolation). Truncation of interpolated results does not affect the interpolation algorithm, but acts as a data filter to control the interpolated result to a specified bound. This may be necessary for estimation of quantities such as percent solids, where concentrations should fit within the range of 5-90%. Another approach is to set the truncation limits to values that are a set percentage of the range above the maximum and below the minimum value in the dataset. A histogram of the dataset can be generated in GMS, and this may be used to provide basis for an allowable range for the interpolation. Truncation of interpolated PCB concentrations to (min, max) values within the extremes of the data range should be avoided, and has not been used in OU1 modeling work.

3.3   Testing Quality Improvement from Dataset Exclusion or Inclusion

Efforts can be directed to scrutinize and rules for the inclusion of archival datasets. In general, newer datasets should outweigh older datasets. One test of improvement should show reduced variability of the determined isosurface volume as the number of data is increased.

Jackknife interpolation can also be used to test the general improvement or deterioration of the interpolation result when a particular dataset is included or excluded. However, the tests should be on the basis of whether regions with PCB concentrations near the RAL are adequately detected, rather than the objective of minimizing raw error at sample locations with higher concentrations.

3.4   Use of Percent Solids as a Covariate Evaluation

Percent solids data and PCBs can be interpolated to the same mesh. In general, percent solids data are correlated with PCB data (low percent solids associated with higher PCB concentrations) and, furthermore, the percent solids data are less spatially variable. Contours of percent solids and TOC can be useful for selecting PCB interpolation methods or designing the mesh, on the basis of correlations. For example, PCB interpolation methods that project the RAL isosurface into sandy regions (high percent solids) should be scrutinized to assess the validity of the model input parameters as, historically, high percent solids values in the Fox River sediments have correlated with low PCB values.

Once the RAL isopach is developed, a new mesh can be generated to better estimate PCB mass and percent solids within the isopach. This may be very useful for the design of dredge and dewatering strategies, and for estimating the benefit in risk-reduction from removal of the PCB mass.

4. Summary

The main objectives of sediment deposit modeling are to accurately delineate regions of PCB contamination and to support remedial design and engineering tasks. The support tasks include dredge prism development, solids estimates, dredge plan guidance, and contingent remedy (capping) appropriateness. 3D modeling of OU1 sediment sub-areas is essential for developing more accurate representations of PCB contaminated sediments at a given RAL by considering the potential correlation of sediment contamination at various depths.

This white paper addresses the rationale, general approach, and refinements used for the selection and application of GMS for sediment modeling in OU1. The two primary modeling tasks having the most significant effect on the results are forming the 3D mesh for the interpolation and selecting the model parameters for accurate delineation of contaminated sediments. These parameters are the number of nearest points, (N_p) to consider for mesh interpolation, and the z-scale anisotropy factor (α_z) to correct for clustering and anisotropy in the vertical direction. Using the GMS implementation of Shepard's IDW method, this white paper evaluates these two primary model parameters.

GMS is shown to be an appropriate 3D model for PCB delineation with adequate flexibility to deal with varying conditions present in OU1, such as varying sediment thickness and large swings in PCB concentrations resulting from depositional dynamics. GMS also contains statistical evaluation tools to assess the accuracy and confidence of the model outputs.

5. References

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