ATTACHMENT 1

MODEL INPUTS

1.0 MODEL INPUT PARAMETERS

Model inputs were derived from extensive site sampling efforts and bench scale testing, as well as literature in some cases. Based on the initial modeling conducted during the FS, as well as analyses conducted since that time, model predictions have been found to be most sensitive to underlying porewater concentration, groundwater upwelling velocity, biological decay rate and sorption parameters (including partitioning to sand cap materials and to GAC amendments). Therefore, an extensive data collection effort and a series of bench-scale evaluations have been ongoing since 2005 to increase understanding and provide site-specific information for these key parameters. The following subsections describe the data collection efforts and basis for developing the input values used for these key model input parameters.

Both deterministic and probabilistic model evaluations were used in developing the chemical isolation layer design. Input parameters for the deterministic simulations were fixed values specified based on the references and rationale provided in detail in Table A1.1. Probabilistic model simulations were completed to assess cap performance against the full range of potential input parameter values (including the “worst-case” values as they pertained to predications of cap performance). Statistical distributions were developed for key input parameters and used in these probabilistic modeling evaluations. The distributions used for such model input parameters, and the basis for their selection (including applicable references and data sources) are also provided in Table A1.1.

1.1 Porewater Concentrations

Multiple sampling methods have been used to measure porewater concentrations within the remediation areas of the Lake. These methods are described further in the Onondaga Lake Phase I Pre-Design Investigation Porewater Methods Evaluation Report (Parsons, 2006). Sampling methods included *in situ* diffusion samplers (peepers), groundwater upwelling pumps and porewater generated via centrifugation of sediment. Peepers and centrifuged samples, in general, produced consistent results and provided readily implementable approaches for collecting a large number of porewater samples. Therefore, data from all three methods (i.e., centrifugation, peepers, and upwelling pumps) were generally used to develop model inputs for pore water concentration.

In consultation with the NYSDEC, correction factors were developed and applied to the porewater data to account for any potential losses during sample collection, handling or analysis. Correction factors varied by compound and sampling methodology. Correction factors for peeper data were based on the results of the Phase II Pre-Design Investigation: Data Summary Report, Appendix J - Diffusion Sampler Equilibrium Study (Parsons, 2009a). For porewater samples generated via centrifugation, correction factors were based on average Matrix Spike/Matrix Spike Duplicate (MS/MSD) recoveries. Groundwater data collected from upwelling pumps in 2002/2003 were discarded, with the exception of mercury and phenol results, due to the potential for losses along the pump tubing. Groundwater data collected from the upwelling pumps, following modification of the tubing during the Phase I Pre-design Investigation (PDI), were incorporated into the model data set without correction factors.[1] Table A1.2 provides a summary of the correction factors employed.

For certain contaminants, the ability to collect porewater samples was limited by the volume required for analysis. Therefore, in the case of PAHs, phenol and PCBs, sediment data from the lake PDI as well as the Remedial Investigation (RI) were used (in conjunction with measurements of TOC, bulk density, and porosity) to calculate porewater concentrations based on equilibrium partitioning equations for use in the modeling effort. Attachment 2 to Appendix B of this design report describes the calculation of porewater concentrations for these compounds.

Initial concentrations used in the model inputs were based on the data selection and calculation methods described above and are further detailed in Table A1.1. Based on the pore water concentration data set for each compound in each model area, empirical distributions were developed. Addendum 1 describes the approach for generating these cumulative distribution functions (CDFs) for each compound in each model area. For deterministic simulations, either the maximum concentration or the best estimate (i.e., mean value) of the distribution was used (as described in Appendix B). Probabilistic modeling was based on sampling from the full distributions. Plots of the full distributions for each compound are provided with the electronic model input files in Appendix B Attachment 5.

1.2 Groundwater Upwelling Velocities

Appendix C to this design report details the field effort and results of the extensive groundwater upwelling investigation conducted on the Lake, and describes the development of the groundwater upwelling inputs that were used in cap modeling. This work was completed to characterize the groundwater upwelling velocities that the sediment cap will be subjected to following construction.

Direct measurements of groundwater upwelling velocity were collected in most of the remediation areas, as detailed in Appendix C. Thus, the measurements of groundwater upwelling velocity collected in the capping areas of Remediation Areas A, E, and in Model Area C2 were used to generate the groundwater upwelling data sets (i.e., empirical CDFs) used in the cap modeling for those areas.

The upwelling rates used in the cap modeling for the four subareas in Remediation Area D, Model Areas B1/C1, B2 and C3 were based on predictions of conditions that would exist once the upland hydraulic containment systems are in place. Estimates of these future upwelling distributions were developed based on calculations of vertical flow through the underlying silt and clay unit based on measurements of thickness, vertical hydraulic conductivity, and hydraulic gradient of that unit in each of these areas. Additional discussion is provided in Appendix C.

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[1] VOC data from groundwater upwelling pumps in the ILWD were inadvertently not included in the model input files, phenol and mercury data from the upwelling pumps was included. These data will be added to the data set during the draft final design, although doing so will not significantly impact the modeling results presented in this design report.

For all modeling areas, the specific upwelling velocities used in the model runs were based on the upwelling velocity distributions developed as described above (i.e., based on empirical data or estimated based on calculations of flow through the slit and clay unit). For deterministic simulations, the best estimate (i.e., mean value) of the distribution was used, and probabilistic modeling was based on sampling from the full distributions, as provided in Appendix C.

1.3 Consolidation Induced Porewater Expression

Settlement calculations indicate that there will be some upward expression of porewater associated with sediment consolidation due to cap placement. This porewater expression would be equivalent to an additional advective flux into the cap during the time that such consolidation occurs. That flux will occur over a relatively short timeframe, after which the long-term conditions represented by the steady-state model would prevail. For steady state model behavior, such an initial expression of porewater does not change the ultimate steady state concentration profile calculated by the model. Therefore, consolidation effects were not included in the steady state analytical modeling. Porewater expression may have a more significant impact on shorter-term performance evaluations of amended cap effectiveness, as simulated with the numerical transient modeling. Therefore, porewater expression was represented in the transient modeling of amended cap areas by adding the calculated pore water flux during the consolidation period to the base upwelling velocity (described above). Appendix E of this design report presents the basis for how predictions of settlement induced porewater expression as a function of time were developed for the purposes of the cap modeling, and Table A1.1 provides more detail on how this process was simulated in the model.

1.4 Sorption Parameters for Sediment and Sand Cap Material

As noted above, porewater concentrations of the sediment beneath the cap used for modeling were based on direct measurements of porewater concentrations, as well as calculations of porewater concentrations from sediment data and partitioning theory, as described in Section 1.1. Partitioning theory was also used to predict partitioning between porewater and sediments beneath the cap and between porewater and the cap materials. The basis for specification of the sorption parameters used in the model is summarized in Table A1.1; details are provided in Attachment 2 to Appendix B of this design report.

1.5 GAC Adsorption Parameters

Site-specific isotherms for various solid media with potential for use as an amendment material were generated for VOCs, mercury and naphthalene during the Phase IV PDI (Parsons, 2009b). Additional isotherm testing for the same list of parameters, with the addition of phenol, was conducted during the Phase VI PDI to validate the Phase IV PDI results and evaluate each isotherm point in triplicate to reduce variability (as compared to the initial testing). Screening studies conducted during the Phase VI isotherm experiments indicated a potential influence of pH on GAC sorption for some compounds. As a result, a second round of isotherms was conducted at neutral pH. Results from the Phase VI adjusted pH isotherms were generally consistent with or more conservative than the Phase IV results. Because of this and the higher levels of QA/QC employed in the Phase VI studies, the Phase VI amended pH GAC isotherms were used in the cap modeling evaluation for all cap areas where a GAC amendment will be used.

GAC isotherm data for PAHs and PCBs were not included in the scope of the site-specific evaluations. In order to model these compounds, the site-specific results for naphthalene were conservatively used to represent PAHs and PCBs. PAHs are composed of multiple benzene rings bonded in a planar configuration. With only two bonded benzene rings, naphthalene is the simplest and smallest of the PAH compounds. All other PAHs consist of greater numbers of bonded benzene rings and are therefore of higher molecular weight, larger molecular size, and greater hydrophobicity; the same is true of PCBs, as these compounds consist of two benzene rings to which between one and ten chlorine atom(s) are bonded. These characteristics all lend themselves to higher relative GAC sorbability than naphthalene. For example, in one study the equilibrium sorbed concentration values for naphthalene and phenanthrene at a water concentration of 0.1 mg/L were determined to be 50 mg/g and 80 mg/g, respectively (USEPA, 1980). Since the addition of each benzene ring (or chlorine atoms in the case of PCBs) will increase the sorptivity relative to naphthalene, applying the site-specific derived Freundlich parameters for naphthalene to the other PAHs and PCBs will yield a highly conservative modeling estimate for the GAC cap amendment.

Model inputs from the Phase VI studies included site-specific Freundlich isotherm parameters (Kf and 1/n) for each compound, as described in Table A1.1. Kf and 1/n values used for the deterministic simulations of each chemical were based on the best estimate for these two parameters as determined through nonlinear regression analysis of the isotherm data. A 95% confidence interval was also generated directly from the experimental data using joint uncertainty bounds for the two parameters in the fitted Freundlich equations (Kf, 1/n). In order to quantify uncertainty around the best estimate of Kf and 1/n for the probabilistic simulations, coefficient pairs were generated by randomly sampling from within these 95% confidence regions.

1.6 Biological Decay

Biological degradation of organic contaminants within the chemical isolation layer is an important contaminant fate process considered in the design of the chemical isolation layer. Over time, natural biological processes will degrade organic contaminants as they slowly migrate upwards into the cap and reduce contaminant concentrations throughout the isolation layer and the overlying habitat layer. Several stages of bench-scale experiments were conducted to evaluate the rate of biological decay anticipated to occur within the cap for key compounds present in lake sediments and porewater (2008, 2009a, 2009c, 2009d).

Rapid decay under aerobic conditions (which will occur within the upper portion of the cap's habitat layer) was consistently observed for all VOCs evaluated, as discussed below. Anaerobic decay was also documented for all VOCs in at least one of the bench-scale studies. However, given the inherent complexities in replicating long-term environmental processes in the relatively short-term laboratory investigation period, it is difficult to quantitatively measure anaerobic biological degradation rates for all of the VOCs. There is evidence from the site-specific testing and in the literature that over time anaerobic biological decay will occur in the isolation cap for all of the VOCs, including naphthalene. However, as a conservative assumption, the current model predictions do not quantitatively incorporate biological decay for of any contaminants, except phenol. Both aerobic and anaerobic biological decay of phenol was observed consistently under a variety of conditions during multiple phases of the PDI bench testing. Therefore, biological decay of phenol was considered in the modeling evaluation in areas that do not require a pH amendment (i.e., Model Areas A1, E1, E2, and E3). Future model evaluations may incorporate biological decay for other contaminants.

2.0 REFERENCES

Parsons. 2006. Onondaga Lake Phase I Pre-Design Investigation: Porewater Methods Evaluation Report. Prepared for Honeywell, Morristown, New Jersey and Syracuse, New York.

Parsons. 2008. Onondaga Lake Pre-Design Investigation: Phase IV Work Plan. Prepared for Honeywell, Morristown, New Jersey and Syracuse, New York.

Parsons. 2009a. Onondaga Lake Pre-Design Investigation: Phase II Data Summary Report, Appendix J – Diffusion Sampler Equilibrium Study. Prepared for Honeywell, Morristown, New Jersey and Syracuse, New York.

Parsons. 2009b. Onondaga Lake Pre-Design Investigation: Phase IV Data Summary Report. Prepared for Honeywell, Morristown, New Jersey and Syracuse, New York

Parsons. 2009c. Onondaga Lake Pre-Design Investigation: Phase III Data Summary Report. Prepared for Honeywell, Morristown, New Jersey and Syracuse, New York

Parsons. 2009d. Onondaga Lake Pre-Design Investigation: Phase V Work Plan. Prepared for Honeywell, Morristown, New Jersey and Syracuse, New York.

USEPA. 1980. Carbon Adsorption Isotherms for Toxic Organics. U.S. Environmental Protection Agency. EPA/600/8-80-023. April 1980.

TABLE A1.1
MODEL INPUT PARAMETERS AND BASIS

Model Input	Site-specific or Literature Based	Reference	Rationale
Initial porewater concentration in underlying sediment: Fixed value (maximum concentration or best estimate (mean) value) used for deterministic simulations. Distribution (CDF) used for probabilistic simulations.	Site-specific	Based on concentrations measured in porewater for the following contaminants: benzene, toluene, ethylbenzene, xylene, chlorobenzene, dichlorobenzenes, trichlorobenzenes, naphthalene, phenol, and mercury (where available). Porewater concentrations for the following contaminants were calculated based on sediment concentrations and equilibrium partitioning formulae: phenol, PAHs, and total PCBs (see Attachment 2). Phenol and mercury data from groundwater upwelling pumps were used, where available, to supplement these values. Data were selected from the following depth intervals: the top 0 to 5 meters in SMU 2 subarea of ILWD, 1 to 5 meters in the West and East subareas of ILWD, 0 to 4 meters in the Center subarea of ILWD, and 0-3 m in Remediation Areas A, B, C and E. Correction factors were applied as appropriate (see Table A1.2). Depth intervals were selected considering the proposed dredge plan and generally include the data from two meters above to two meters below the maximum dredge cut in an area, exclusive of hot spot dredging in the ILWD. This is conservative because it includes data from sediments that will be dredged, which generally contain higher porewater contaminant concentrations than the remaining sediments. Under Honeywell’s proposed approach, no removal is proposed in portions of the ILWD Center and ILWD West subareas. For the ILWD West subarea, porewater data from depths of 1 to 5 meters were used to generate an area-wide data set. Data from the top meter in the ILWD West subarea were excluded as this layer will be removed over a significant portion of that subarea. Concentrations in the top meter are	Spatial variability exists across the Lake capping areas. The ILWD has been broken into four subareas to account for larger-scale differences in contaminant concentration distributions. Likewise, Remediation Areas A, B, C and E have each been separated into smaller Modeling Areas: A1, A2, B1/C1, B2, C2, C3 and E1, E2, E3 based on differences in porewater concentration. Probabilistic simulations were based on empirical cumulative distribution functions developed from the concentration datasets for each CPOI within a given modeling area; CDFs are provided in Attachment 5. Further explanation of the development of the CDFs is provided in Addendum 1.

Model Input	Site-specific or Literature Based	Reference	Rationale
		generally lower than or consistent with the deeper porewater data, and therefore exclusion of these data does not have a significant impact on the porewater distribution used in the modeling. *Honeywell Onondaga Lake Locus Database, 2010.*	
Molecular diffusion coefficient: Fixed value	Literature	Fixed value by compound. *Lyman, W.J, Reehl, W.F. and Rosenblatt D.H. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, D.C.*	Little to no spatial variability or uncertainty anticipated.
Hydrodynamic dispersivity: Fixed value	Literature	Conservative value fixed at 10% of the total cap thickness. Homogenous cap layer expected to exhibit significantly smaller dispersivity. *Domenico and Schwartz (1990), Physical and Chemical Hydrogeology, John Wiley.*	Upper bound employed, not expected to significantly impact cap design.
Partition coefficient (Koc / Kd) for isolation sand and underlying sediment: Fixed value used for VOCs in deterministic simulations (best estimate – mean value). Distribution used for VOCs in probabilistic simulations.	Site-specific for VOCs and mercury Literature for PCBs, PAHs, and phenol	Log Koc values for VOCs (mean and standard error[2]) calculated using regression of paired sediment/porewater measurements from Phase I-VI data. Normal distribution of log Koc specified based on these values for probabilistic simulations. Paired data were also used for estimating mercury Kd's in the native sediments (for use in numerical modeling) *See Attachment 2.* Literature value used for phenol based on *NYSDEC Technical Guidance for Screening Contaminated Sediment (NYSDEC,*	The variability observed is likely due to sampling methodology and analytical limitations. To evaluate the impact of this variability, the distribution for log Koc is modeled by a normal distribution defined by the mean and standard error, with the standard error representing uncertainty about the mean value. For the literature-based values used for PAH, PCB, and phenol modeling, uncertainty was not represented, since there

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[2] The uncertainty in the mean is characterized by the standard error, as opposed to the standard deviation which characterizes the variability of individual values. Therefore, distributions used in the probabilistic analysis were mostly normal or lognormal distributions developed using the mean and the standard error (= standard deviation / sqrt (number of observations)) of the data (or the log transformed data in the case of a lognormal distribution).

Model Input	Site-specific or Literature Based	Reference	Rationale
For mercury, phenol, PCBs, and PAHs: a fixed value was used for all simulations		*1999)).* Values used to represent partitioning to cap material for PAHs and PCBs based on NYSDEC screening guidance values; corrected literature values to represent partitioning in underlying sediment, as described in *Attachment 2*. Mercury partitioning coefficients for sand based on data from: Reible, D., 2009. *Phase IV Addendum 2 Report –Isotherm Experiments with Organic Contaminants of Concern with Sand, Organoclay and Peat and for Mercury with Sand, Organoclay, Peat and Activated Carbon.*	is no information available to estimate site-specific variation in the values derived from NYSDEC Guidance.
Porosity (isolation and habitat layers): Fixed value	Literature	Fixed value of 0.4. Theoretical maximum porosity for uniform spherical particles is 0.4765 (cubic packing); if the particles are rhombohedrally packed, then the uniform maximum porosity is 0.2595. Baseline value based on a typical value for loosely packed, medium-grain sand.	Little to no spatial variability or uncertainty anticipated. Given the relatively small % by weight or volume of GAC that will be present in the isolation layer the value of 0.4 is also appropriate for the bulk mixed media. In places where the habitat layer will consist of gravel material, use of this value is also appropriate because: 1) the porosity of typical gravel material would likely only be slightly lower than this value; and 2) the model is not sensitive to such small differences in porosity. For example, Domenico and Schwarz (1990) list the following ranges of porosity values for sands and gravels:

Model Input	Site-specific or Literature Based	Reference	Rationale
			• Gravel, coarse: 0.24 to 0.36 • Gravel, fine: 0.25 to 0.38 • Sand, coarse: 0.31 to 0.46 • Sand, fine: 0.26 to 0.53
Porosity (underlying sediment): Fixed value	Site-specific	Average porosity in area modeled (A1, E1, E2, etc.) calculated from sediment samples collected in that area. *Honeywell Onondaga Lake Locus Database, 2010.*	The critical model input parameter is the initial porewater concentration (Co), which was either measured or calculated from sediment data. Since the calculated value is a function of sediment characteristics such as fraction organic carbon, porosity and particle density (along with sediment contaminant level), it is difficult to coherently apply distributions to all these parameters simultaneously. The decision was made to prioritize Co, and use fixed values for the underlying sediment characteristics. Using a fixed value for porosity is not expected to significantly impact cap design.
Particle density of sand cap material (un-amended isolation layer and habitat layer) and underlying sediment : Fixed value	Literature	Fixed value of 2.6 g/cm^3 *Freeze, R.A., Cherry, J.A. 1979. Groundwater. Prentice-Hall, Inc., Englewood Cliffs, New Jersey.*	Little to no spatial variability or uncertainty anticipated. Not expected to significantly impact cap design. This value is appropriate for either a sand or gravel habitat layer.

Model Input	Site-specific or Literature Based	Reference	Rationale
Particle density of GAC-amended isolation layer: Fixed value	Design parameter	The transient numerical model was developed to primarily simulate a sorptive amendment as a thin layer that consists entirely of amendment material (i.e., placement as a mat). In order to simulate a bulk mixture of sand and GAC in a single layer, the input parameters for the "active layer" in the model are specified such that the thickness of the layer equals the thickness of the bulk media, and that the specified thickness, along with the input values for particle density and porosity of that layer, result in the desired GAC application rate. For example, to achieve a GAC application rate of 0.3 lb/ ft^2 over a 12" layer of bulk sand and GAC, the following are specified for model inputs in that layer: • thickness: 30.48 cm • porosity: 0.4 • particle density: 0.008 g/cm^3 and the resulting GAC application rate is: $(0.008\ g/cm^3) * (1-0.4) * (30.48\ cm) * (1\ lb / 453.6\ g) * (30.48\ cm / ft)^2 = 0.3\ lb/ft^2$ Essentially, the particle density accounts only for the mass of GAC amendment in the layer. Setting the parameters in this way implicitly (and conservatively) assumes that the sand material in the isolation layer has no sorptive capacity.	Value for each amended cap area determined as part of design to establish recommended GAC application rate.
foc (isolation layer and habitat layer below bioturbation zone): Fixed value	Site-specific	Model input value based on the average foc of 0.022% (222 mg/kg) measured in samples of the sand cap material during the Phase VI PDI. *Honeywell Onondaga Lake Locus Database, 2010.*	Little to no spatial variability or uncertainty anticipated. This value for foc is also applicable in the habitat layer below the bioturbation zone. In areas where the habitat layer will consist of gravel materials

Model Input	Site-specific or Literature Based	Reference	Rationale
			the foc is anticipated to be minimal, so this value is applicable for gravel habitat layer material as well.
foc (underlying sediment): Fixed value	Site-specific	Average values calculated from individual sediment sample results collected in each modeling area. *Honeywell Onondaga Lake Locus Database, 2010.*	The critical model input parameter is the initial porewater concentration (Co), which was either measured or calculated from sediment data. Since the calculated value is a function of sediment characteristics such as fraction organic carbon, porosity and particle density (along with sediment contaminant level), this makes it difficult to coherently apply distributions to all these parameters simultaneously. The decision was made to prioritize Co, and use fixed values for the underlying sediment characteristics. Using a fixed value for the underlying sediment foc is not expected to significantly impact cap design.
foc (bioturbation zone of habitat layer): Fixed value (best estimate) for deterministic simulations, distribution for probabilistic simulations	Site-specific	Normal distribution based on mean and standard error of site-specific (ln-transformed) TOC data in the top six inches of lesser-impacted non-ILWD SMUs (SMU 4 and 5), length weighted averages were developed for cores where multiple sample intervals were collected in the top 0-6" . *Honeywell Onondaga Lake Locus Database, 2010.*	Inherent uncertainty exists in trying to estimate the ultimate post-remedy TOC that will be established in the upper layer of the sediment cap. Site-specific data may provide a suitable estimate of this input parameter in areas of the lake not impacted (or impacted to a lesser degree) by METRO processes and Solvay Waste materials, both of which tend to produce higher TOC values. To address the uncertainty around future TOC levels in the upper layer of the

Model Input	Site-specific or Literature Based	Reference	Rationale
			cap data in the 0-6" interval from SMUs 4 and 5 were used to develop a range of surficial TOC. The SMU 4/5 data do not exhibit any spatial structure and are expected to be an overestimate of post-remedy TOC given recent decreases in organic loading and lake productivity associated with METRO upgrades. This data set was described by a lognormal distribution represented by the mean and standard error. This value for foc is based on the assumption that clean sediment will be deposited in the habitat layer over time. This assumption is not impacted by the application of a sand or gravel habitat layer material.
Freundlich coefficients for GAC: Fixed value (best estimate based on nonlinear regression of isotherm data) for deterministic simulations Distribution for probabilistic simulations based on sampling from 95% joint confidence	Site-specific	Isotherm experiments were conducted by Carnegie-Mellon to establish sorption characteristics of the proposed activated carbon to be used. Parsons conducted a series of isotherm experiments during the Phase VI PDI to verify the Carnegie Mellon results, reduce variability through analysis of triplicate samples, and account for impacts of neutralized pH. Model inputs were based on the Phase VI isotherm data *Draft Report for the Phase VI Addendum 1 PDI will be submitted in January 2010.* Naphthalene isotherm parameters were conservatively used to represent isotherm parameters for PAHs and PCBs.	The best estimates of Kf and 1/n (as determined by nonlinear regression of the isotherm data) were used for deterministic model runs. In order to quantify uncertainty around the mean values used for Kf and 1/n, a 95% confidence region was generated around the means, and estimates of the coefficient pairs randomly taken from within that range were used for the probabilistic simulations. The 95% confidence interval was generated directly from experimental data (a two parameter (Kf, 1/n) nonlinear sorption isotherm).

Model Input	Site-specific or Literature Based	Reference	Rationale
region.			
Boundary layer mass transfer coefficient: Fixed value	Site-specific	Fixed value of 0.363 cm/hr. Eqn 11 of *Thibodeaux and Becker, 1982 (4 m/s windspeed, 5m water depth, benzene, 500m fetch). Thibodeaux, L. J., and Becker, B., (1982). "Chemical transport rates near the sediment of a wastewater impoundments", Environmental Progress, Vol 1; no. 4, p 296-300.*	Little to no spatial variability or uncertainty anticipated.
Particle biodiffusion coefficient (bioturbation zone of habitat layer): Fixed value (best estimate) for deterministic simulations. Distribution for probabilistic simulations.	Literature	Normal distribution of log transformed values. *Thoms, S.R., Matisoff, G., McCall, P.L., and Wang, X. 1995. Models for Alteration of Sediments by Benthic Organisms, Project 92-NPS-2, Water Environment Research Foundation, Alexandria Virginia*	Uncertainty associated with size, depth and distribution of benthic organisms. Data from freshwater sites employed to generate a lognormal distribution.
Porewater biodiffusion coefficient (bioturbation zone of habitat layer): Fixed value (best estimate) for deterministic simulations. Distribution for probabilistic	Literature	Normal distribution based on mean and standard error of log transformed values derived from literature. *Wood, L.W. (1975) Role of oligochaetes in the circulation of water and solutes across the mud-water interface. Verhandlungen der Internationalen Vereinigung fur Theoretische und Angewandte Limnologie. 19: 1530-1533. Svensson, J.M., and L. Leonardson. (1996) Effects of bioturbation by tube-dwelling chironomid larvae on oxygen uptake and denitrification in eutrophic lake sediments. Freshwater Biology. 35: 289-300. Cunningham (2003) Unpublished PhD dissertation, Louisiana State University, D. Reible, Advisor.*	Uncertainty associated with size, depth and distribution of benthic organisms. Data from freshwater sites employed to generate a lognormal distribution.

Model Input	Site-specific or Literature Based	Reference	Rationale
simulations.			
Darcy velocity: Fixed value (best estimate – mean value) for deterministic simulations. Distribution for probabilistic simulations.	Site-specific	Site-specific groundwater upwelling data used to generate an empirical cumulative distribution function for the data sets in Model Areas A1, A2, C2 and Remediation Area E (Model Areas E1, E2, and E3 combined). Upwelling velocities used in Remediation Areas B, C (excluding Model Area C2) and D were based on the best estimate of conditions that would exist once the upland hydraulic containment systems are in place. To represent these anticipated conditions in the cap modeling, a probabilistic simulation approach was used to calculate a distribution of upwelling velocities within each modeling area. These simulated distributions were generated based on the variations in hydraulic conductivity, hydraulic gradient, and thickness of the underlying clay layer, and were found to closely follow lognormal distributions, which formed the basis of the model inputs. Further detail is provided in Appendix C. In all cases, the best estimate (i.e., mean value) of the distribution was used for deterministic simulations, and probabilistic modeling was based on sampling from the full distributions (empirical CDF or lognormal), as provided in Appendix C.	Simulation of separate sub-areas and model areas (with the exception of Remediation Area E as described below) captures major spatial variation in upwelling rate (resulting from differences in underlying clay thickness and underlying sediment/soil structure). The impacts of smaller-scale variations in upwelling within these subareas/model areas are quantified by the probabilistic results (i.e., the distribution in outputs captures measurement uncertainty as well as spatial variability). No significant spatial variability was observed within Remediation Area E; thus, data from the three model areas were pooled and used to specify the same CDF for each individual area. Additional discussion on Groundwater data sets used in the modeling is provided in Appendix C.

Model Input	Site-specific or Literature Based	Reference	Rationale
Biological decay rate (isolation and habitat layers): Fixed value	Site-specific	For phenol, a conservative value of 75 days (half life) was used based on the Phase V batch tests. Rapid aerobic decay was observed for all VOCs evaluated during the PDI (see Section 4 of the main document). Given the inherent complexities in replicating long-term environmental processes in the relatively short-term investigation period, it was difficult to quantitatively demonstrate consistent anaerobic biological degradation for the organic contaminants of concern for quantitative model simulations. There is evidence from the testing to date (see Section 4 of the main document) and in the literature that over time anaerobic biological decay is likely to occur in the isolation cap for most or all of the VOCs, including naphthalene. However, quantifying and employing explicit rates of biological degradation and designing the isolation cap based on those assumptions is uncertain given the limited ability to replicate biological processes anticipated to occur over hundreds to thousands of years. Therefore, as a conservative assumption, the current model predictions do not consider biological decay of the 23 CPOIs, benzene or toluene. *Interim Report on Phase V PDI Biotreatability Study Interim Report submitted in July 2010.*	Biotreatability testing conducted in 2009 and 2010 provided limited data on the biodegradation rates for phenol. Phenol analysis was conducted at the start of the test and after 82 days (Group A) and 78 days (Group B). The degradation rates calculated from these data are considered conservative (i.e., suggesting slower degradation or a longer half lives) because: 1) the analysis of the data does not incorporate an acclimation period prior to more rapid biodegradation; and 2) the concentration of phenol in some of the microcosm bottles dropped below the detection limit before the time the second sample was collected. Additional testing is underway to refine this estimate. A conservative value for the biodegradation half-life of phenol at 12 C was specified based on the average of the half-lives for the two tests conducted at 12 C (105 and 45 days/ treatments 17A and 20A), which is equal to 75 days. A distribution for phenol was not required as probabilistic modeling was not conducted in non-amended cap areas (A1 and E1) and biological degradation was not represented in the probabilistic modeling of amended cap areas.
Consolidation induced porewater expression: Fixed	Site-specific	For each remediation area, a power function was used to represent the cumulative consolidation-induced pore water flux over time. These functions were developed based on the best	Values selected to represent best estimate of the total porewater flux associated with consolidation and timeframe over which

Model Input	Site-specific or Literature Based	Reference	Rationale
value that varies over time		estimates of total consolidation flux (primary and secondary) and the timeframe over which approximately 90% of the total is reached, within each Remediation Area. The total consolidation ranges from 0.5 ft (Remediation Area D) to 3.2 ft (Remediation Area B). The time to reach 90% of those values varies from 15-20 years (Remediation Area D) to ~1 year (Remediation Area A). The time-derivative of the resulting consolidation vs. time curve is used by the model to calculate a time-varying upwelling velocity that is added to the base-upwelling rate input to the model. This process was modeled over a 30-year timeframe (because at longer times, the incremental upwelling velocity becomes negligible). Details are provided in Appendix E.1 for non-ILWD areas and in Appendix E.2 for the ILWD.	such consolidation would occur in each remediation area based on settlement estimates, as described in Appendix E.

TABLE A1.2
CORRECTION FACTORS FOR POREWATER CONCENTRATIONS

Porewater Sample Collection Method	Correction Factor
Peepers (Phases I, II & III)	
Xylenes (total)	1.1
Chlorobenzene	1.1
Toluene	1.1
Ethylbenzene	1.1
Benzene	1.1
1,3-Dichlorobenzene (phases I & II)	1.2
1,3-Dichlorobenzene (phase III)	1.1
1,4-Dichlorobenzene (phases I & II)	1.2
1,4-Dichlorobenzene (phase III)	1.1
1,2-Dichlorobenzene (phases I & II)	1.2
1,2-Dichlorobenzene (phase III)	1.1
Naphthalene (phases I & II)	1.2
Naphthalene (phase III)	1.1
Mercury (Tuffryn)	1.1
1,2,4-Trichlorobenzene (phases I & II)	1.2
1,2,4-Trichlorobenzene (phase III)	1.1
1,2,3-Trichlorobenzene (phases I & II)	1.2
1,2,3-Trichlorobenzene (phase III)	1.1
1,3,5-Trichlorobenzene (phases I & II)	1.2
1,3,5-Trichlorobenzene (phase III)	1.1
Centrifuge (Phases I, II, III & IV)	
Xylenes (total)	1.11
Chlorobenzene	1.11
Toluene	1.08
Ethylbenzene	1.07
Benzene	1.09
1,3-Dichlorobenzene	1.10
1,4-Dichlorobenzene	1.14
1,2-Dichlorobenzene	1.15
Naphthalene	1.54
Mercury	1.06
1,2,4-Trichlorobenzene	1.45
1,2,3-Trichlorobenzene	1.53
1,3,5-Trichlorobenzene	1.07

ADDENDUM 1

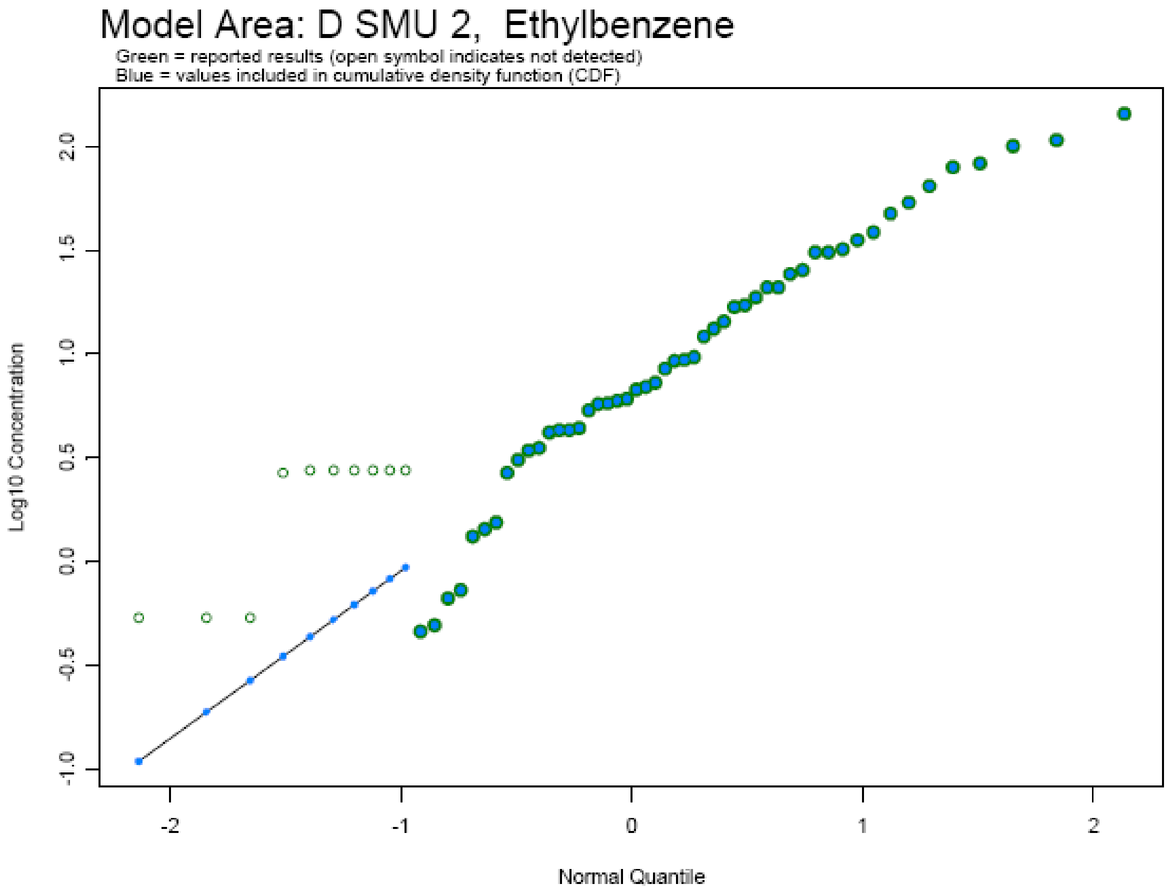
CUMULATIVE DISTRIBUTION FUNCTIONS FOR POREWATER CONCENTRATION

The contaminant concentrations in the porewater of the sediments underlying the cap were characterized by data collected in Onondaga Lake. There were certain cases where the presence of a relatively high proportion of non-detect results introduced uncertainty at the lower end of the concentration distribution. For example, Figure A.1 shows the distribution of ethylbenzene concentrations in SMU 2, with non-detect sample concentrations plotted at the detection limit (5 ug/L) as green open symbols. Clearly, assuming all non-detect results are equal is inappropriate, whether at the detection limit which would be overly conservative or at zero which is equally inappropriate.

The approach used to estimate the full distribution of contaminant concentrations was based on the observation that the detected concentrations generally follow a log-normal distribution (that is, the detected data are roughly linear in Figure A.1); thus a reasonable and logical assumption is that the non-detect concentrations follow this same distribution. A cumulative distribution function was derived based on the detected concentrations, and this function was then used to estimate values for the non-detect results. Specifically, a truncated log-normal distribution was fit to only the detected concentrations by fitting a linear regression to predict log-concentration from the normal z-score values (i.e., a regression through the green filled symbols was used to generate the resulting black line in Figure A.1). Z-score values were assigned assuming all of the detected concentrations were higher than the non-detect sample results. The fitted regression line was then used to predict log-concentrations for the normal z-score values attributed to the non-detect samples (see open symbols in Figure A.1). Finally, the empirical cumulative distribution function was used to characterize the distribution of porewater concentrations for the probabilistic simulations, restricted to the range of detected and estimated concentrations. This approach is recommended by Ginevan and Splitstone 2004.

Figure A.1

Ethylbenzene concentrations in the porewater of sediment from SMU2



Reference:

Ginevan, Michael E., and Douglas E. Splitstone, 2004. Statistical tools for environmental quality measurement. CRC Press LLC. p. 229.