

MEMORANDUM

To: Caryn Kiehl-Simpson, Parsons **Date:** January 18, 2011
From: Deirdre Reidy, Anchor QEA, LLC **Project:** 090139-01.20
Kevin Russell, Anchor QEA, LLC
Re: Onondaga Lake Cap Modeling Files for Intermediate Design Report

This memorandum details the files and directory structure associated with the cap modeling that was performed as part of the Onondaga Lake Dredging, Capping, and Habitat Intermediate Design Report. The cap modeling files are organized into three main folders:

1. Steady State Model
2. Numerical Model
3. Porewater Cumulative Distribution Functions (CDFs)

The remainder of this memorandum describes the files and subfolders contained in each folder.

STEADY STATE MODEL

The steady state model is located in the `|SS_Model|` folder. Several changes to the model have been made since the Initial Design Submittal (IDS), including:

- One MS Excel file (*Steady_State_Model_1201_2010.xlsx*) is used to simulate all chemicals and model areas.
 - There is tab corresponding to each model area.
 - For a given model area, all chemicals are modeled on the same tab—one column per chemical.
 - The model runs deterministic simulations only. The Monte Carlo functionality has been stripped from the model and therefore @Risk is not required.
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The *Master I-O* tab of the Excel spreadsheet contains the main model inputs and outputs. It begins with the model outputs, and the inputs start at row 106. Inputs are organized first by those that vary by both area and chemical, then those that vary by chemical only, followed by those that vary by area only, and finally global inputs (for which single values apply to all chemicals and areas). Cell *B106* is used to set the porewater concentration statistic used for simulating the chemicals (i.e., maximum or average concentration). Similar to the model file used for the IDS, the input values from the *Master I-O* tab are linked to the individual model area/chemical calculations by formulae. Likewise, the outputs from each of the area-specific tabs are linked back to the Output section of the *Master I-O* spreadsheet, so that all outputs can be viewed in one place.

NUMERICAL MODEL

The numerical model files are contained in three subfolders:

1. Model Code
2. Inputs
3. Outputs

The contents of each of these folders are described in this section.

Model Code

Deterministic Modeling

Three Matlab® files are used to run deterministic simulations with the numerical model. These files are located in the *Numerical_Model\ModelCode\numerical_deterministic* folder. The main code files, *parsons_MC_consolidation_VOCs.m* and *parsons_MC_consolidation_PCBs_PAHs_Hg.m* (which are slightly different versions of the model used to simulate volatile organic compounds (VOCs) and polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), and mercury (Hg), respectively as described below), both call the function *consolidation.m*.

The user can control which areas are simulated, as well as file paths for model input and output files, by modifying the *parsons_MC_consolidation_VOCs.m* code as follows:

- Line 48 is where the model areas are specified.
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- Line 49 is where the path to the input files is specified.
- Line 54 is where the path for the output files is specified.
- Lines 57 to 100 are where the chemicals to be simulated for each area are specified.

For simulating PCBs, PAHs, and Hg, an additional line of code is modified by the user in the *parsons_MC_consolidation_PCBs_PAHs_Hg.m* file (to specify whether average or maximum porewater concentrations were used for the simulation):

- Line 56 is where the porewater concentration statistic is specified (either “Avg” for average concentration or “Max” for maximum concentration).

Probabilistic Modeling

Three Matlab® files are used to run the probabilistic (Monte Carlo) numerical model. These files are located in the *Numerical_Model\ModelCode\numerical_probabilistic* folder.

The main program, *parsons_MC_consolidation.m*, calls the two functions: *consolidation.m* and *freundlichrand.m*. Similar to deterministic simulations, the user controls which model areas are simulated and input/output file paths by modifying the code as follows:

- Line 48 is where the model areas are specified.
- Line 49 is where the path to the input files is specified.
- Line 53 is where the path for the output files is specified.
- Lines 56 to 79 are where the chemicals to be simulated for each area are specified.

Numerical Model Inputs

The input files used for simulations with the numerical model are located in the *Numerical_Model\Inputs* folder. One input file is used for each model area; the same file is used for both deterministic and probabilistic simulations. Each input file contains one tab per chemical modeled. Each file contains an *Input_Matrix* tab, which is where the inputs for the various model parameters are specified. The granular activated carbon (GAC) application rate is entered by the user in cell *B12*. In addition, drop-down menus in cells *B16* and *B17* are used to select the porewater concentration statistic used for the simulations (i.e., maximum or average concentration). The chemical-specific tabs each use formulae to fill in the appropriate model inputs based on the values specified in the *Input_Matrix* tab, for the

given model area and chemical specified in cells *C6* and *B7* of the chemical-specific tabs, respectively.

Numerical Model Outputs

Deterministic Model Outputs

The model output files from deterministic simulations are located in the *Numerical_Model\Outputs\Det_Output* folder. Within this folder, outputs for each model area are contained in separate folders, and within those folders results for PAHs and Hg are stored in subfolders aptly named *PCBs_PAHs_Hg* (where applicable). The outputs are saved in the comma-delimited format (*.csv). Output file names follow a naming convention that helps to understand the model scenario:

“Output_”<Model Area> “_” <Chemical Name Abbreviation> “_” <GAC application rate>

For file naming purposes, the GAC application rate component of the file name does not include a decimal point. It should be understood that the decimal place is located between the first and second digits. For example, *Output_B1C1_B_05.xls* is the file containing the outputs from the model simulation of benzene in area B1/C1 with 0.5 lb/sf GAC, and similarly, *Output_C2_N_0005.xls* is the file containing the outputs from the model simulations of naphthalene in area C2 with 0.005 lb/sf GAC. As the PAHs and Hg underwent a secondary set of conservative model simulations that involved running the model using maximum initial porewater concentrations, the PAH and Hg output files also include in the filename the term “Max” or “Avg” to specify the concentration statistic that was used for the simulation. No such label was used for VOCs, since all deterministic simulations with the numerical model were based on average porewater concentrations.

Probabilistic Model Outputs

The probabilistic model output files are located in the *Numerical_Model\Outputs\MC_Output* folder. Within this folder, outputs for each model area are contained in separate folders, and within those folders results for PAHs and Hg are stored in subfolders aptly named *PCBs_PAHs_Hg* (where applicable). The probabilistic

model output file names follow the same naming convention used for deterministic simulations described above.

The probabilistic model outputs are saved in two formats: MS Excel (*.xls) and comma-delimited format (*.csv). The comma-delimited format is a duplicate of the last eight columns of the MS Excel output (to facilitate rapid evaluation of results), except that the blank cells (meaning 1000+ years for times to probable effects concentration [PEC] exceedance) in the *.xls version are replaced with “NaN” in the *.csv version.

POREWATER CUMULATIVE DISTRIBUTION FUNCTIONS

The folder *|Porewater_CDFs|* contains files related to the development of porewater CDFs. The sample locations and concentration data used for generating these CDFs are contained in a series of Excel files located in this folder. The resulting CDFs (i.e., numerical concentration values and their corresponding cumulative frequency intervals) are contained in the file *CDFoutput.xls*, and PDF files showing plots of the resulting CDFs that were generated for each area and chemical are also located in this folder.
