OTIS-MCAT Quick Start Guide

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Project GitHub Site:
https://github.com/WardHydroLab/OTIS-MCAT.git

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PART 1 – DEMO

The OTIS-MCAT is bundled with sample output files from the associated publication. By executing the file “OTISMCAT.m” in Matlab, the following operation should be expected:

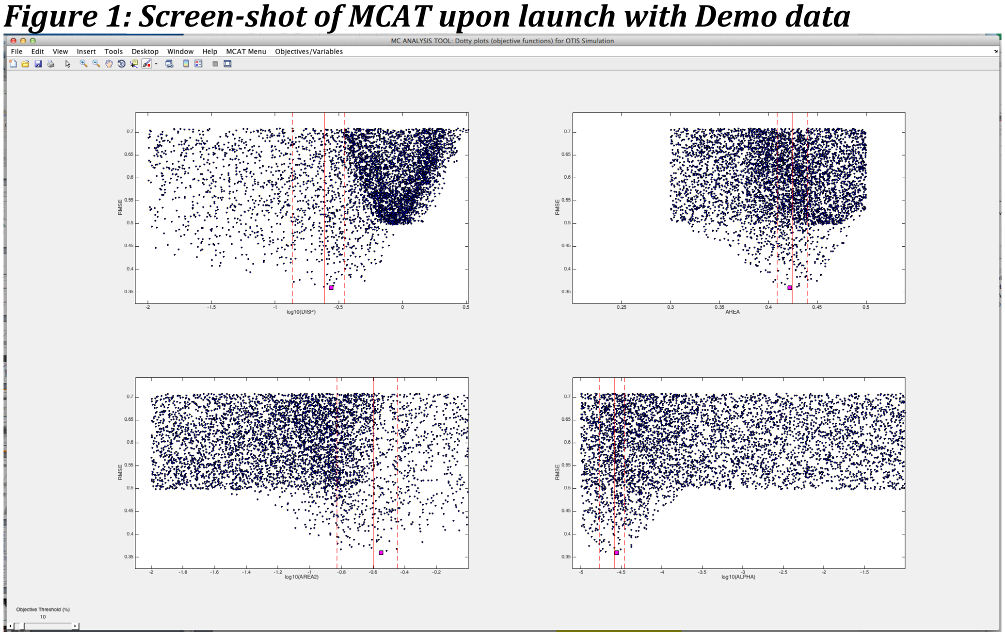
(1) The following lines will be printed to the Matlab Command Window (providing status updates on the execution of the code and various options):

```
Run Start: 23-Mar-2016 10:38:50
OTIS_MCAT_CONTROL.txt read correctly
upstream.csv read correctly
downstream.csv read correctly
Results Saved as BTCAnalysis.csv
Monte Carlo runs not requested
Simulations not conducted, attempting to load
existing output files
MCRunData.mat loaded successfully
BTCs.mat loaded successfully
All metrics being input to MCAT
MCAT input files built successfully
Creating and saving boxplots
Creating and saving CI distributions
OTIS-P *.out files already exist
No OTIS-P files were written
Launching MCAT - OTISMCAT.m run complete
Run End: 23-Mar-2016 10:39:02
```

(2) A series of four multi-boxplot figures (similar to Figure 7 in the associated manuscript) and four confidence interval figures (similar to the rows of Figures 5 and 8 with y-axis labeled “Frequency”) will be displayed, saved, and closed. The folders “Boxplots” and “CI_plots” will be added to the “Output_files” directory, and the images saved as *.eps files.

(3) The MCAT will open, displaying four dotty plots:

Figure 1: Screen-shot of MCAT upon launch with Demo data



(4) At this point, users are free to interact with the MCAT and analyze the data. To explore the MCAT interface, we suggest:
    a. Use the "Objectives/Variables" to select a different objective function. The dotty-plots should automatically update.
    b. Use the slider bar in the bottom-left corner, labeled "Objective Threshold (%)" to change what fraction of the results are plotted. 10% is the default, indicating the dots represent the top 10% of solutions based on the selected objective function.
    c. Use the "MCAT Menu" to explore different visualizations of the data, re-creating some figures from the associated manuscript. We suggest to explore:
        i. Dotty Plots Objective Function (the default visualization)
        ii. A Posteriori Parameter Distribution
        iii. Identifiability Plot
        iv. Regional Sensitivity Analysis
    d. Notes on the user interface
        i. The "Objectives/Variables" menu, "MCAT Menu", and "Objective Threshold (%)" can be adjusted in any order desired.
        ii. Some additional MCAT tools will not work with the default data set because too many objective functions are present (e.g., multi-objective plots, simulation pixel plots, time-series surface plots). See discussion of Line 64 in Part 2.
        iii. Some additional MCAT tools require additional analyses to be completed, which can be time consuming (e.g., PARETO Output Uncertainty, DYNIA

(5) An "echo" file of the command line is stored as "Output_files/OTISMCATecho.txt"

(6) A summary of the metrics calculated for the observed breakthrough curve is saved as "Output_files/BTCAnalysis.csv"

PART 2 – EXECUTION OF YOUR OWN OTIS-MCAT RUNS

STEP 1: Download and the OTIS-MCAT code from GitHub
Download the OTIS-MCAT code distribution as a *.zip file, and extract the files on your machine in a working directory.

GitHub Site: https://github.com/WardHydroLab/OTIS-MCAT.git

STEP 2: Download the appropriate OTIS executable file
Execution of the OTIS-MCAT requires that an executable version of the OTIS code that is compiled for your machine is available and located in the correct directory. Bundled with the code on GitHub are executable files for UNIX and Microsoft Windows 64-bit operating systems. Additional executable files are available for download from the USGS at:
http://water.usgs.gov/software/OTIS/

Users should verify that the executable works on their machine by carefully reviewing the OTIS documentation from the USGS, and successfully executing Example 1 in the sample files available with the OTIS download.

To verify that the executable already bundled with the software will work on your machine, it is suggested to test the appropriate executable in the folder "code/OTIS-MCAT_TEST/" (either OTIS.EXE for Windows OS, or otis for UNIX).

The key outcome of STEP 2 is that working OTIS executable is placed in the folder "code/OTIS-MCAT_TEST/", with a filename matching exactly the existing executable files.

*****If the OTIS executable does not work on your machine (i.e., if you cannot complete Example 1 in the OTIS downloads from the USGS), OTIS-MCAT will not work correctly*****

STEP 3: Build the required input files
Templates are provided with the code download. The files and their preparation are detailed below.

upstream.csv – time-series of in-stream concentration at the upstream end of the solute tracer study. This is commonly the data observed at the well-mixed location downstream of the injection. Note that times should be specified in hours. It is recommended to prepare this file using a spreadsheet tool or write-out the data from another computer program.

downstream.csv – time-series of in-stream concentration at the downstream end of the study reach. Same preparation and formatting instructions as the ***upstream.csv*** file.

OTIS_MCAT_CONTROL.txt – the primary input file to specify model options and parameter ranges. It is recommended to edit this file in a plaintext editor (e.g., TextEdit, TextPad, TextWrangler) rather than a WYSIWYG editor (e.g., MS Word, Pages). Line-by-line specifications of the inputs and relevant notes are presented in this section. A sample input file is displayed for reference in Figure 2.

Figure 2. Example input file for OTIS-MCAT.

OTIS_MCAT_CONTROL.txt

```
%--------------------------------------------------------------------------------
% SYSTEM CONFIGURATION, ACTIONS
%--------------------------------------------------------------------------------
1       ;% OS (1 = Windows, 2 = UNIX)
0       ;% Run MC Simulations? (1 = yes, 0 = no)
1       ;% Launch MCAT? (1 = yes, 0 = no)
0       ;% Show waitbar while simulations are being calculated? (1 = yes, 0 = no)
%--------------------------------------------------------------------------------
% BASIC MODEL CONTROLS SET IN THIS SECTION
%--------------------------------------------------------------------------------
15      ;% dt - timestep for calculations (s)
1       ;% dx - spatial step for calculations (m)
0.0125  ;% Qstart - discharge at upstream end of model (m3/s)
581     ;% Length of study reach between observation points (m)
50000   ;% Number of Parameter Sets to test in simulation
0       ;% Random seed (0 = use clock; any positive integer = re-createable)
%--------------------------------------------------------------------------------
% OTIS PARAMETERS AND RANGES
%--------------------------------------------------------------------------------
1e-2    ;% DISP minimum value (m2/s)
10      ;% DISP maximum value (m2/s)
1e-5    ;% ALPHA minimum value (s-1)
1e-1    ;% ALPHA maximum value (s-1)
1e-2    ;% A_S minimum value (m2)
1       ;% A_S maximum value (m2)
2       ;% AREAFLAG (1 = estimate area & specify relative bounds; 2 = specify range)
0.1     ;% AREA minimum value, (if AREAFLAG = 1, as AGUESS*__ ; if AREAFLAG = 2, AMIN m2)
1.0     ;% AREA maximum value, (if AREAFLAG = 1, as AGUESS*__ ; if AREAFLAG = 2, AMAX m2)
%--------------------------------------------------------------------------------
% DISCHARGE PARAMETERS AND RANGES
%--------------------------------------------------------------------------------
0.0015  ;% Minimum lateral inflows for the reach (m3/s)
0.0015  ;% Maximum lateral inflows for the reach (m3/s)
0       ;% Minimum lateral outflows for the reach (m3/s)
0       ;% Maximum lateral outflows for the reach (m3/s)
0       ;% Minimum lateral inflow C for the reach (g/m3)
0       ;% Maximum lateral inflow C for the reach (g/m3)
%--------------------------------------------------------------------------------
% DECAY PARAMETERS AND RANGES
%--------------------------------------------------------------------------------
0       ;% Minimum value for lambda: in-stream first order decay (s-1)
0       ;% Minimum value for lambda: in-stream first order decay (s-1)
0       ;% Minimum value for lambda2: storage zone first order decay (s-1)
0       ;% Minimum value for lambda2: storage zone first order decay (s-1)
%--------------------------------------------------------------------------------
% SORPTION PARAMETERS AND RANGES
%--------------------------------------------------------------------------------
0       ;% Minimum value for lambda hat (s-1)
0       ;% Maximum value for lambda hat (s-1)
0       ;% Minimum value for lambda hat 2 (s-1)
0       ;% Maximum value for lambda hat 2 (s-1)
0       ;% Minimum value for rho (g/m3)
0       ;% Maximum value for rho (g/m3)
0       ;% Minimum value for Kd (m3/g)
0       ;% Maximum value for Kd (m3/g)
0       ;% Minimum value for Cbackground (mg/L)
0       ;% Maximum value for Cbackground (mg/L)
%--------------------------------------------------------------------------------
% CONTROL OF MODEL OUTPUTS
%--------------------------------------------------------------------------------
1       ;% Output full BTCs? (0 = no; 1 = yes)
1       ;% Output metric-parameter box plots? (0 = no; 1 = yes)
10      ;% Default percentage of results to include in outputs? (e.g., 10 = 10%)
0       ;% Which metrics to feed into MCAT? (0 = all metrics, 1 = select a list of 10)
1       ;% Output plots of CIs? (0 = no; 1 = yes)
```

SYSTEM CONFIGURATION, ACTIONS. These inputs control which modules in the OTIS-MCAT are executed, and which complied OTIS code is used for simulations.

Line 4 – specify the operating system of your machine. Current options are "1" for Windows and 2 for UNIX.

Line 5 – optional to execute or skip the execution of the Monte Carlo simulations. If simulations have been previously run, specify 0 to skip re-running and simply launch the MCAT. If simulations have not been run, or you desire to re-run the simulations, specify 1.

Line 6 – specify 1 to launch the MCAT upon completion of the Monte Carlo simulations (if requested on Line 6). Specify 0 to skip launch of MCAT tool.

Line 7 – specify 1 for an interactive waitbar to be displayed during Monte Carlo simulations. Specify 0 to suppress this visualization.

NOTE – for execution of the Monte Carlo simulations, users may with to use a high-performance computer or "cluster" computer available on their campus. For this case, set lines 6-7 to 0 to suppress visualizations, which commonly cause errors in command-line UNIX commands issued on these systems.

BASIC MODEL CONTROLS SET IN THIS SECTION. These inputs control the geometry and time steps used in the OTIS model.

Line 11 – computational time step for OTIS (s)

Line 12 – spatial increment for OTIS (m)

Line 13 – discharge at the upstream end of the study reach (m^3 s^{-1})

Line 14 – total distance between the locations where upstream.csv and downstream.csv were observed (m)

Line 15 – number of parameter sets to generate for the Monte Carlo simulations

Line 16 – random seed option. Specifying a value of 0 uses the current time and date as the seed for the random number generator in Matlab, providing true randomization of data. For most users, a value of 0 will be sufficient. Specifying any positive integer uses that value to "seed" (i.e., initiate) the random number generator. Users who wish to use the same random distribution for multiple data sets should specify a non-zero value.

OTIS PARAMETERS AND RANGES. These inputs control the physical transport processes to be simulated within OTIS. For each parameter, set the minimum and maximum values to an identical value to fix that value. All parameter values must be positive (non-zero) for the code to properly run.

Lines 20-21. Specify minimum and maximum values for in-stream longitudinal dispersion (m^2 s^{-1}).

Lines 22-23. Specify minimum and maximum values for fractional stream-storage exchange coefficient (s^{-1}). To remove the impacts of transient storage from the simulations, set these values to an infinitesimally small non-zero value (e.g., 1E-20).

Lines 24-25. Specify minimum and maximum values for cross-sectional area of the transient storage domain (m^2).

Line 26. Specify one of two options for area calculations.

For a value of 1:

area is estimated based on discharge, stream distance, and the modal transit time observed in the specified upstream.csv and downstream.csv files. Use this option if the area range is unknown.

For a value of 2:

area is specified in the same format as other parameters. Use this option if you know the range of areas you want to consider.

Lines 27-28.

For Line 26 = 1:

specify the relative range of areas to explore around the estimate described in the previous section. Specified values are used to define the minimum and maximum areas as:

$A_{min} = A_{estimate}$ * Line 30

$A_{max} = A_{estimate}$ * Line 31

As an example, entering values of 0.5 and 1.5 results in exploring a range of areas ranging from 50 to 150% of the estimated value.

For Line 26 = 2:

specify minimum and maximum cross-sectional area of the stream.

DISCHARGE PARAMETERS AND RANGES. These inputs control the lateral inflows and outflows to be simulated within OTIS. For each parameter, set the minimum and maximum values to an identical value to fix that value. All parameter values must be positive (non-zero) for the code to properly run. To omit a parameter from the study, set both maximum and minimum values to zero.

Lines 32-33. Specify the range of lateral inflows to the study reach (m^3 s^{-1}). Lateral inflows are distributed evenly along the length of study reach defined on Line 15.

Lines 34-35. Specify the range of lateral outflows to the study reach ($m^3\ s^{-1}$). Lateral outflows are distributed evenly along the length of study reach defined on Line 15.

Lines 36-37. Specify the range of lateral inflow concentrations to the study reach (g m^3), associated with the inflow rates specified on lines 38-39.

DECAY PARAMETERS AND RANGES. These inputs control first order decay of the solute to be simulated within OTIS. For each parameter, set the minimum and maximum values to an identical value to fix that value. All parameter values must be positive (non-zero) for the code to properly run. To omit a parameter from the study, set both maximum and minimum values to zero.

Lines 41-42. Specify the range of main channel first order decay coefficient (s^{-1}).

Lines 43-44. Specify the range of storage zone first order decay coefficient (s^{-1}).

SORPTION PARAMETERS AND RANGES. These inputs control the streambed and hyporheic sorption and desorption processes to be simulated within OTIS. For each parameter, set the minimum and maximum values to an identical value to fix that value. All parameter values must be positive (non-zero) for the code to properly run. To omit a parameter from the study, set both maximum and minimum values to zero.

Lines 48-49. Specify the range of main channel sorption rate coefficient (s^{-1}).

Lines 50-51. Specify the range of storage zone sorption rate coefficient (s^{-1}).

Lines 52-53. Specify the range of sediment mass accessible per volume of water (g m^{-3}).

Lines 54-55. Specify the range of distribution coefficients for sorption ($m^3\ g^{-1}$).

Lines 56-57. Specify the range of background storage zone concentration (g m^{-3}).

CONTROL OF MODEL OUTPUTS. These inputs control what is automatically stored from the Monte Carlo runs and the MCAT.

Line 61. Specify 1 to store the full simulated solute tracer breakthrough curves at the downstream end of the study reach, or 0 to omit them. Storing the full breakthrough curves may generate large output files, but is required for several of the MCAT tools (e.g., DYNIA). These tools are included in the software but not discussed in detail in the manuscript.

Line 62. Specify 1 to automatically generate a series of boxplots comparing model results for all possible objective functions, after Figure X in the manuscript, automatically stored in the folder “Output_files/boxplots”. Specify 0 to skip this output. Boxplots are only generated for all objective functions being loaded into Matlab (i.e., Line 64 = 1).

Line 63. Specify the default fraction of model runs, in percentage, to include in when MCAT is launched, and for visualization in the boxplots (line 62).

Line 64. Specify which objective functions to load into the MCAT. A value of 0 loads all objective functions. However, some MCAT functions that are included in the software but not specifically detailed in the manuscript (e.g., multi-objective plots, simulation pixel plots, time-series surface plots) do not work with too large of a number of objective functions. Specifying a value of 1 will request the user to interactively specify up to 10 metrics on the command line prior to launching the MCAT.

Line 65. Specify 1 to automatically generate a series of confidence interval plots for the RMSE objective function (similar to the rows of Figures 5 and 8 with y-axis labeled “Frequency”). Figures are automatically stored in the folder “Output_files/CI_plots”. Specify 0 to skip this output.

STEP 4: Execute Monte Carlo Simulations

With input files created, OTIS-MCAT is run by executing the file “OTISMCAT.m” from the Matlab command line. It is advisable to execute a small test-case of 100-1000 runs to test the software and troubleshoot any limitations on your machine prior to execution of a large suite of Monte Carlo simulations. Upon completion of the simulations, the parameter values and objective functions will be stored in the *.mat files in the folder “Output_files”.

STEP 5 (OPTIONAL): Integration with OTIS-P

OTIS-MCAT is designed to interface with OTIS-P. When the code is run to launch the MCAT, the code will automatically complete one of the following steps:

> ***IF*** OTIS-P has been run and the input and output files placed in the folder “OTIS-P_files” (detected by the presence of “star.out” in that folder),
> ***THEN*** code will load the OTIS-P results from the file “star.out” and display the final best-fit OTIS-P parameters and the associated 95% confidence intervals on dotty plots produced in the MCAT.
>
> ***IF*** OTIS-P has not been run (i.e., if “star.out” is not located in the “OTIS-P_files” folder),
> ***THEN*** the input files required to execute OTIS-P will be automatically created and stored in the folder “OTIS-P_files”. At this point, users could readily

execute OTIS-P, and repeat STEP 5 to launch the MCAT and read-in the OTIS-P results for visualization.

STEP 6: Launch MCAT
If line 6 was set to a value of 1 when the code was executed, output visualizations (boxplots as set on Line 62, confidence interval plots as set on Line 65) and OTIS-P files (if OTIS-P has not yet been run) will be generated.

Recommended workflow

(1) Build input files from field data
(2) Run and store the Monte Carlo simulations (Line 5 = 1, Line 6 = 0), including storage of the full solute breakthrough curves (Line 61 = 1).
(3) Use the files placed in the folder "OTIS-P_files" to work through an OTIS-P parameter optimization, as described in the OTIS model documentation. Place all files used for the final OTIS-P run and the associated outputs in the folder "OTIS-P_files".
(4) Launch the MCAT to analyze the already-stored data (Line 5 = 0, Line 6 = 1). Include both box-plots (Line 62 = 1) and confidence interval plots (Line 65 = 1). We recommend first sending all metrics to the MCAT (Line 64 = 0).
(5) If additional MCAT functionality is desired (e.g., multi-objective plots, simulation pixel plots, time-series surface plots), set Line 64 = 1 and select the metric(s) desired for further analysis. Suppress box-plot and confidence interval outputs (Line 62 = Line 65 = 0).