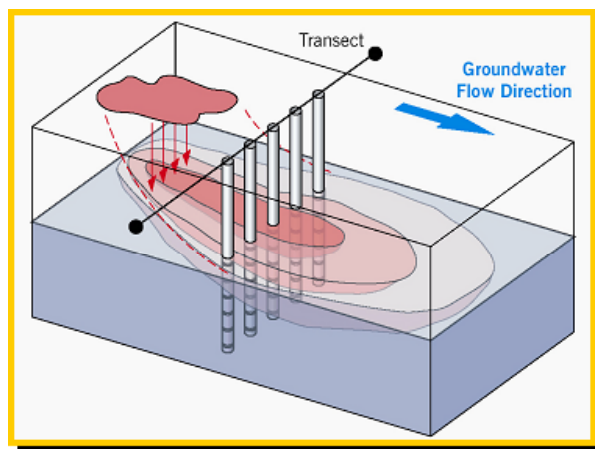


Mass Flux Toolkit

To Evaluate Groundwater Impacts,
Attenuation, and Remediation Alternatives



USER'S MANUAL

Version 1.0
March, 2006

By

S.K. Farhat, Ph.D. and C.J. Newell, Ph.D., P.E., DEE
Groundwater Services, Inc.
Houston, Texas

Eric M. Nichols
LFR Levine-Fricke
Newfields, New Hampshire

Report Documentation Page				Form Approved OMB No. 0704-0188	
Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.					
1. REPORT DATE MAR 2006		2. REPORT TYPE		3. DATES COVERED 00-00-2006 to 00-00-2006	
4. TITLE AND SUBTITLE Mass Flux Toolkit To Evaluate Groundwater Impacts, Attenuation, and Remediation Alternatives. User's Manual				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Groundwater Services, Inc.,2211 Norfolk St. Suite 1000,Houston,TX,77098				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT Same as Report (SAR)	18. NUMBER OF PAGES 135	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			



DISCLAIMER

The Mass Flux Toolkit is made available on an as-is basis without guarantee or warranty of any kind, expressed or implied. The United States Government, Groundwater Services, Inc., the authors and reviewers accept no liability resulting from the use of the Mass Flux Toolkit or its documentation. Implementation of the Mass Flux Toolkit and interpretation of the predictions of the model are the sole responsibility of the user.

MASS FLUX TOOLKIT TO EVALUATE GROUNDWATER IMPACTS, ATTENUATION, AND REMEDIATION ALTERNATIVES

ENVIRONMENTAL SECURITY TECHNOLOGY CERTIFICATION PROGRAM

TABLE OF CONTENTS

Section	Page No.
DISCLAIMER	A
INTRODUCTION	1
INTENDED USES FOR MASS FLUX TOOLKIT AND LIMITATIONS	4
MASS FLUX TOOLKIT MODELS.....	6
<i>Mass Flux Transect Calculator</i>	<i>6</i>
<i>Uncertainty Analysis</i>	<i>9</i>
<i>Impact of Mass Flux.....</i>	<i>10</i>
MASS FLUX TRANSECT CALCULATOR	11
<i>Mass Flux Transect Calculator Data Entry</i>	<i>12</i>
<i>Input Data and Grid.....</i>	<i>14</i>
<i>Method for Interpolating Grid</i>	<i>24</i>
<i>Grid Completion</i>	<i>25</i>
<i>Mass Flux Results.....</i>	<i>27</i>
<i>Final Concentration Grid.....</i>	<i>29</i>
<i>Mass Flux Summary</i>	<i>31</i>
<i>Uncertainty Analysis</i>	<i>32</i>
RECEPTOR IMPACT WORKSHEETS.....	35
<i>Receptor Impact - Wells.....</i>	<i>36</i>
<i>Receptor Impact - Streams.....</i>	<i>39</i>
<i>API Strategies Tool.....</i>	<i>41</i>
CURRENT ESTCP/SERDP MASS FLUX PROJECTS	42
REFERENCES	43
MASS FLUX TOOLKIT TROUBLESHOOTING TIPS	46
<i>Minimum System Requirements.....</i>	<i>46</i>
<i>Installation and Start-Up</i>	<i>46</i>
<i>Spreadsheet-Related Problems.....</i>	<i>46</i>
<i>Common Error Messages.....</i>	<i>46</i>
ACKNOWLEDGEMENTS	48

TABLE OF CONTENTS

APPENDICES	50
APPENDIX A.1. PROBABILITY DISTRIBUTIONS	51
<i>A.1.1 Normal Distributions</i>	<i>51</i>
<i>A.1.2 Lognormal Distributions</i>	<i>51</i>
<i>A.1.3 Uniform Distributions</i>	<i>52</i>
APPENDIX A.2. LATIN HYPERCUBE SAMPLING	53
EXAMPLES	55
EXAMPLE 1: MASS FLUX CALCULATION	56
EXAMPLE 2: MTBE CONCENTRATION AT CONTROL POINT	66
CASE STUDY	69
CASE STUDY: MTBE AND TBA	70

INTRODUCTION

Traditional site investigations have focused on collecting both chemical concentrations and subsurface flow characteristics. These data have typically been analyzed separately, such as when chemical concentrations are compared to regulatory standards. When the two types of data are combined, it is typically for use in solute transport models.

Recently there has been increased emphasis on combining chemical and flow data into a single metric to provide estimates of contaminant mass flux. This flux is the rate that a contaminant passes through a defined cross section in units of mass per time. Although the strict definition of mass flux is mass discharge per unit area (in units of mass per time per area), many researchers and practitioners use the term *mass flux* to denote the rate of “mass discharge” or “total mass discharge”. *This document will use the term “mass flux” to represent data in units of mass per time passing by a plume transect perpendicular to groundwater flow.*

Regulatory acceptance of this approach, and the number of sites where mass flux has been used, are rapidly increasing. More research and industry groups (U.S. EPA, 1998; Devlin *et al.*, 2002; Connecticut, 2002; Rao *et al.*, 2002; Newell *et al.*, 2003; ASTM, 1998, Kavanaugh *et al.*, 2003) suggest that a mass flux approach may provide key insights about how groundwater plumes behave and how they should be managed. For example:

The USEPA’s Scientific Advisory Board (U.S. EPA, 2001) recommended that:

“In summary, measurements of mass flux of the contaminants and footprint parameters – not just concentrations - are necessary to document cause-and-effect and to assess long-term sustainability/permanence. Site-characterization and monitoring plans should be proactively designed to accommodate mass-flux estimates.”

Pankow and Cherry (1996) state that:

“Therefore, the ultimate impact of plumes emanating from solvent DNAPL source zones can be evaluated in terms of impact of relatively small annual mass fluxes to the receptor such as water-supply wells or surface waters. In some cases, the fluxes present significant risk to human health and/or the environment, and extensive remedial action is warranted. In other cases, the fluxes are insignificant, and remedial action would provide little or no actual environmental risk reduction.”

Despite the interest in using the mass flux approach, calculating mass flux from field data is not easy. There are several methods to choose from, each with its own strengths and limitations. The most commonly used method, calculating mass flux from transect data, remains a difficult and laborious process. The concentration data is multiplied against the corresponding flow area data to give flux for a specific cross-sectional area of the plume. The results from all the flow areas are summed together to obtain a mass flux across the transect. However, few groundwater monitoring networks provide data that offer a straightforward calculation of mass flux (Figure 1). Rather, a transect drawn across a plume often intersects monitoring locations at different lateral spacings, and each well may have a unique screened interval. Hydraulic characteristics determined by aquifer tests are rarely defined at all wells, and can vary from one well to the next. Thus, a consistent evaluation of mass flux may require a significant amount of analysis time and effort.

Other methods, such as extraction well capture and in-situ flux meters are less common. There is a need for increased tech transfer information on how to apply these new technologies.

There are several methods that use mass flux data for site assessment and plume management. Einarson and MacKay (2001a) present simple dilution calculations based on mass flux estimates for plumes and pumping rates from wells that capture this mass flux. The American Petroleum

Institute's (API) "Groundwater Remediation Strategies Tool" (Newell *et al.*, 2003) provide a useful framework for using mass flux for making site management decisions, but the key worksheets from this product will only be available in a paper form.

Finally, there is a concern that mass flux estimates can have significant uncertainty (Kavanaugh *et al.*, 2003). For example, Fraser *et al.*, (2005) evaluated mass flux vs. sampling density for a naphthalene plume at the Borden research aquifer. When the sampling grid density was reduced from 1.7 points per meter squared to 0.7 points per meter squared, the range (as a standard deviation) in mass discharge increased to more than 50%. Guilbeault *et al.* (2005) showed that 75% of the mass flux occurred within 5% to 10% of the transect cross section area for three plumes in Ontario, New Hampshire and Florida, and that a spacing no larger than 15 to 30 cm was needed at some locations to identify high concentration zones.

To help site managers and site consultants estimate mass flux and understand the uncertainty in those estimates, the Environmental Security Technology Certification Program (ESTCP) of the U.S. Department of Defense (DoD) has funded the development of a computerized Mass Flux Toolkit (Toolkit).

The Mass Flux Toolkit is an easy-to-use, free software tool that gives site personnel the capability to compare different mass flux approaches, calculate mass flux from transect data, and apply mass flux to manage groundwater plumes. In this software, the term **mass flux** is used to describe the mass discharge rate in a groundwater plume in units of mass per time passing across a plume transect.

The software, programmed in the Microsoft® Excel spreadsheet environment, provides the following tools to calculate and evaluate mass flux of contaminants in groundwater:

1) Calculation of Mass Flux

A module to calculate the total mass flux across one or more transects of a plume and plot mass flux vs. distance to show the effect of remediation/impact of natural attenuation processes. Three types of uncertainty analysis are included: uncertainty range due to interpolation; uncertainty due to the variability in the input data using a Monte-Carlo like analysis; and an uncertainty analysis that shows how dependent the mass flux estimate is on data from each monitoring point.

2) Impact of Mass Flux

A module allowing users to perform critical dilution calculations for plumes approaching production wells or streams. An additional feature calculates the capture zone of the supply well, directing the user to alter the transect dimensions if the transect does not encompass the capture zone.

3) Learn About Mass Flux

- A module that provides a review of theory and methods of estimating mass flux.
- a. *Overview of Mass Flux Calculations*: a module that provides information about different mass flux calculation methods;
 - b. *Uncertainties in Mass Flux Estimates*: a module that provides information about the main sources of uncertainty associated with mass flux estimates;
 - c. *Emerging Mass Flux Resources*: a review of the emerging mass flux methods;
 - d. *Extraction Well Capture Summary*: a review of theory and methods of estimating mass flux from a pumping well or wells that fully capture a contaminant plume;
 - e. *In-Situ Flux Meter Summary*: a detailed explanation of this emerging mass flux method;
 - f. *Computer Model Resources*: an outline of how commonly available, public domain models such as BIOSCREEN and BIOCHLOR can be used to obtain mass flux estimates at several points in a plume;

INTRODUCTION

- g. API Groundwater Remediation Strategies Tool:* an electronic version of the American Petroleum Institute's (API) Groundwater Remediation Strategies Tool to help users apply mass flux to groundwater remediation decision making.

The Mass Flux Toolkit was developed for the Environmental Security Technology Certification Program (ESTCP) by Groundwater Services, Inc., Houston, Texas.

INTENDED USES FOR MASS FLUX TOOLKIT AND LIMITATIONS

The **Mass Flux Toolkit** attempts to assist site managers and site consultants perform mass flux calculations more quickly and cheaply, permitting their inclusion in more evaluations of groundwater plumes. With mass flux data, the progress of natural attenuation and remediation systems can be demonstrated more vividly and directly to regulators, making the entire remediation process clear, effective, and efficient.

The **Mass Flux Toolkit** is intended to be used in four ways:

1. **As a tool for calculating mass flux and performing dilution calculations.** The Toolkit can be used to help estimate the mass flux using the transect method. Although other mass flux estimation techniques are emerging, the transect method is an established technology. The Toolkit brings together key technical resources, easy-to-use calculation worksheets, and case studies together in one easy-to-access platform.
 - a. In addition, the Toolkit provides three methods for analyzing uncertainty in the total mass flux estimates derived from the transect method. One option utilizes the Monte Carlo type approach to analyze uncertainty in the actual concentration, hydraulic conductivity, and gradient measurements. With this tool, groundwater practitioners can estimate the accuracy of the hydrologic measurements that are being used for the mass flux calculation.

The second option provides a tool for estimating the contribution of each individual observation to the total mass flux. If a single monitoring point represents a high percentage of the total mass flux, then the uncertainty in the calculation is high and additional monitoring points should be added to reduce the uncertainty.

The third method shows the uncertainty involved in the interpolation scheme that is used to calculate mass flux.
 - b. The Toolkit can also be used to perform critical dilution calculations for plumes approaching production wells or streams. An additional feature calculates the capture zone of the supply well and compares it to the transect used to calculate the mass flux, directing the user to alter the transect dimensions if the transect does not encompass the capture zone.
2. **As a data management system for storing and interpreting mass flux data.** Many sites will continue to be monitored for a long period of time. Data from this monitoring program can be stored in MAROS (Monitoring and Remediation Optimization System, a data management system, <http://www.gsi-net.com/software/MAROS.htm>) and then used to update remediation timeframe data. This database function can be used to calculate, store, and compare mass fluxes for different time periods.
3. **As a tool for identifying what information is needed to reduce the uncertainty in mass flux estimates.** Applying the Toolkit to a site can help users identify what types of data are required to improve the mass flux estimates and reduce the uncertainty in the estimate.

4. **As a tool for learning about and comparing various methods of calculating mass flux.** The Toolkit reviews emerging mass flux methodologies with an emphasis on data requirements, applications, advantages, and disadvantages of each approach.

In summary, the software will give site personnel the capability to compare different mass flux approaches, calculate mass flux from transect data, and apply mass flux to manage groundwater plumes. With this tool, site personnel will be able to perform mass flux calculations more quickly and cheaply, permitting their inclusion in more evaluations of groundwater plumes. With the mass flux data, the progress of natural attenuation and remediation systems can be demonstrated more vividly and directly to regulators, making the entire remediation process clear, effective, and efficient.

The Toolkit has the following assumptions and limitations:

- The Toolkit assumes the user is familiar with basic groundwater transport and mass balance concepts.
- The Toolkit assumes uniform flow and concentration throughout each grid cell.
- The Toolkit assumes that the plume top, bottom, and sides are known.
- The Toolkit assumes that the sampling network is dense enough to characterize the structure of the plume. Fraser *et al.*, (2005) and Guilbeault *et al.* (2005) show that monitoring networks need to have a very extensive system of monitoring points to capture the heterogeneity of the plume in the Y-Z plane. This means that mass flux estimates can have significant uncertainty.
- To run the Monte Carlo analysis, users need to estimate what type of statistical distribution best fits the input data and what values best describe the distribution. In many cases there will not be data to make these estimates, so the user may have to rely on scientific/engineering judgment to use the Monte Carlo analysis.
- The Monte Carlo analysis cannot account for plume data that are not part of the monitoring system. Actual mass flux values can be outside the range of the reported range of mass flux values from the Monte Carlo analysis (for example, if new data shows high concentration zones that were not captured by the original monitoring network).
- The capture zone module does not adjust the mass flux based on the degree of capture, but only provides information on the estimated size of the capture zone.

MASS FLUX TOOLKIT MODELS

The Mass Flux Toolkit software has models for calculating mass flux and determining its impact on plumes approaching a stream or supply well.

Mass Flux Transect Calculator

The Toolkit calculates the total mass flux across one or more transects of a plume, using the transect approach, and plots mass flux vs. distance to show the effect of remediation/impact of natural attenuation processes. The information presented in this section is obtained directly from the API's "Groundwater Remediation Strategies Tool" (Newell *et al.*, 2003):

Estimation of mass flux across one or more transects through an affected groundwater plume involves the following principal steps:

1. **Characterize Plume Concentrations:** For each selected plume transect, sufficient groundwater sampling points must be available to define i) the full width and thickness of the plume and ii) the distribution of contaminant concentrations within the plume. Either single-level or multilevel groundwater monitoring points may be used for this purpose. Multilevel monitoring points can provide a more detailed three-dimensional characterization of contaminant concentrations in groundwater. However, single-level groundwater monitoring networks, while less accurate than multi-level networks, can still provide sufficient accuracy to support a mass flux analysis at many sites.

(NOTE: an alternative method is to use the concentrations from contour lines as measurement points. The locations where the transect intersects contour lines from plume maps can be used to construct flow areas for the mass flux calculations).

2. **Characterize Groundwater Flow:** To characterize the specific discharge (q) across each plume transect, representative measurements are required for both the hydraulic flow gradient (i) and the hydraulic conductivity (K) of the flow system (where $q = K \times i$). The groundwater flow direction and hydraulic gradient for each segment of a transect line can be determined from a potentiometric surface contour map based on static water level measurements of available sampling points. Representative measurements of the hydraulic conductivity of the groundwater-bearing unit should be obtained at one or more locations, using appropriate slug test or pumping test methods.
3. **Select Plume Transects:** To characterize mass flux, transects should be located at points where sufficient data are available to define affected groundwater concentrations and specific discharge, as defined in Steps 1 and 2 above. For two-dimensional data (i.e., from single-screen monitoring wells), the transect will represent a line extending across the full width of the plume, perpendicular to the direction of groundwater flow (see Figures 1 and 2). For uniform flow fields, this transect will be a straight line, but, for converging or diverging flowlines, the transect will be curvilinear in shape. For three-dimensional data (i.e., from multilevel monitoring wells), the transect line will represent a vertical plane through the groundwater plume, positioned perpendicular to groundwater flow (see Figures 3 and 4).

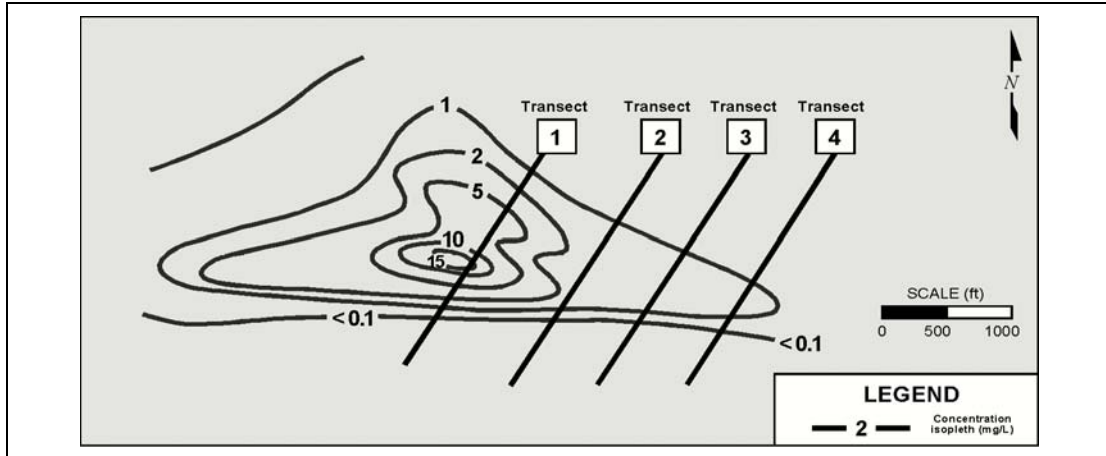


Figure 1. Example Transects through 2-D Plume Contour Map, Dover AFB, Delaware (Adapted from: Einarson, 2001)

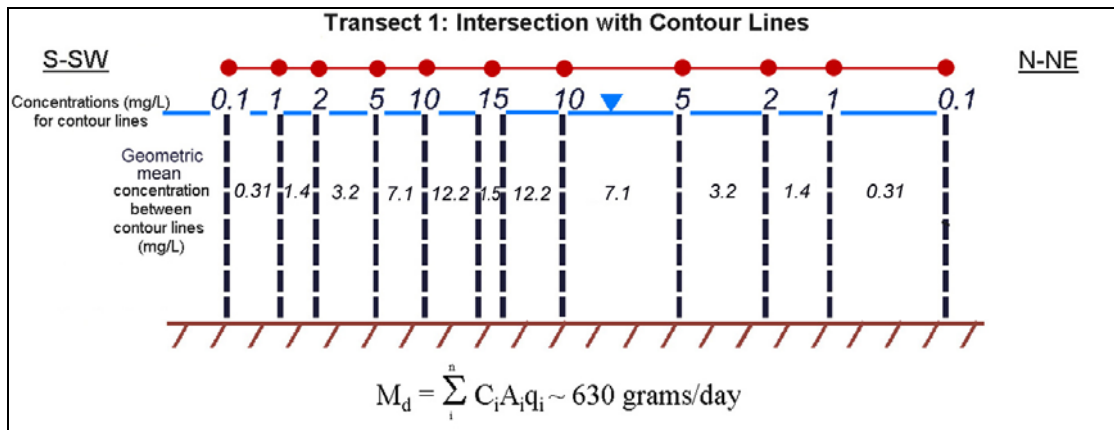


Figure 2. Concentration Profile for 2-D Transect No. 1 Based on Concentration Contours Shown in Figure 2 (Adapted from: Einarson, 2001)

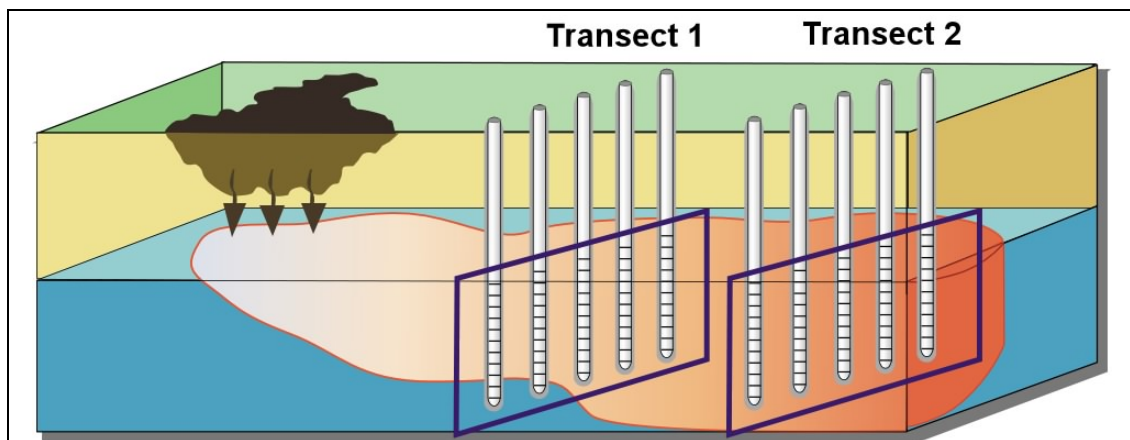


Figure 3. Example Transects through 3-D Plume Delineation

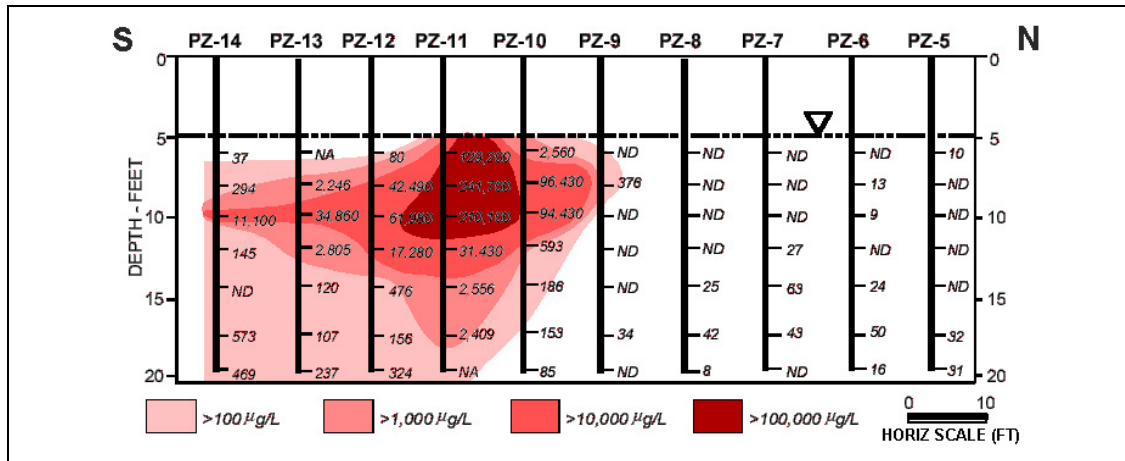


Figure 4. MTBE Concentration Profile for 3-D Transect No. 1
(Adapted from: Einarson, 2001)

4. Subdivide Transects Into Subareas: Each transect should be divided into subareas. Typically, each subarea represents a different concentration value. Two methods are commonly applied. For Method 1, subareas are divided to represent the area between concentration isopleths on a contour map of the plume. The concentration is assumed to be the geometric mean of the two contour values. For Method 2, sufficient monitoring points are located directly on the transect to construct transect subareas. The dividing line between subareas is typically halfway between the measurement points. In some cases, a combination of Method 1 and Method 2 can be applied. For three-dimensional transects, the transect plume should be subdivided into polygons bounded by contour data (Method 1) or centered on available measuring points (Method 2) (See Figures 3 and 4 for an example of Method 2).

5. Calculate Cumulative Mass Flux Across Transect: The total contaminant mass flux across the transect is calculated as follows:

$$w = \sum_{i=1}^{i=n} C_i q_i A_i CF$$

where:

w = total mass flux from source zone (g/day) (also called mass discharge)

C_i = concentration of constituent at flow area in transect (mg/L)

q_i = specific discharge (also called Darcy velocity) through flow area associated with an individual constituent measurement i (cm/sec). q_i can be calculated using:

$$q_i = K \cdot i$$

where:

K = hydraulic conductivity (cm/sec)

i = hydraulic gradient (cm/cm)

A_i = Flow area associated with an individual constituent measurement (ft²)

CF = conversion factor = 80.3 (ft/cm)/(sec/day)(L/ft³)(g/mg)

Guidelines for selecting key input parameters for the model are outlined in [Mass Flux Transect Data Entry](#). For help on results see [Mass Flux Transect Results](#).

Uncertainty Analysis

Uncertainty in mass flux estimates is a key issue in using mass flux as a metric. There are three main sources of uncertainty in a mass flux estimated from transect data:

Type 1: Uncertainty in the actual concentration, hydraulic conductivity, and gradient measurements. Uncertainty in the water quality data (concentration) can be estimated by evaluating temporal trends over time and evaluating the amount of data scatter. Groundwater practitioners can estimate the accuracy of the hydrologic measurements (hydraulic conductivity and hydraulic gradient) that are being used for the mass flux calculation.

Type 2: Uncertainty in the interpolation scheme. Different interpolation schemes will result in different mass flux estimates. Some interpolation schemes, such as kriging, provide local estimates of uncertainty, however, kriging is not be used in the Toolkit. The effect of the different interpolation schemes can be addressed by performing the mass flux calculation with the different schemes included in the Toolkit.

Type 3: Uncertainty associated with unmeasured values. This type of uncertainty is related to Type 2 uncertainty. However, the uncertainty associated with areas of high mass flux that are missed by the monitoring scheme is difficult to assess.

The Toolkit provides options for characterizing Type 1 uncertainty quantitatively using two features: Monte Carlo analysis and crossvalidation. Guidelines for selecting key input parameters for the model are outlined in [Uncertainty Analysis](#). Type 2 uncertainty is handled by calculating mass flux with all possible interpolation schemes, and showing the range in the resulting mass flux estimates.

The Toolkit calculates Type 2 uncertainty in mass flux for the Nearest Neighbor, Linear Interpolation, and Log Transformation for any grid that requires interpolation (except User Interpolated) and plots the minimum and maximum values as error bars on the Mass Flux Summary sheet.

Simple Uncertainty Analysis (Spatial Uncertainty Analysis)

The Toolkit applies crossvalidation to evaluate the uncertainty in the sampling point location. Crossvalidation is a method of removing one observation at a time, estimating a value for the removed observation using the remaining observations, and calculating the output (Olea, 1999). The removed value is then replaced and the next observation removed. This process is continued until all the observations have been removed one at a time. The Toolkit will remove each observed value of concentration, hydraulic conductivity, and gradient one at a time during crossvalidation.

Advanced Uncertainty Analysis (Input Uncertainty Analysis)

Monte Carlo analysis is a method of analyzing and quantifying uncertainties in model outputs due to the uncertainties in the input parameters (Rong *et al.*, 1998). Monte Carlo analysis refers to a computer based system that uses random numbers from a probability distribution to obtain an approximation for the parameter of interest (U.S. EPA, 1997; Bergin and Milford, 2000).

In the standard Monte Carlo approach, simple random sampling, a large number of runs (typically 100 to 1000) are required to obtain a meaningful probability distribution for the parameter. For each run of the standard approach, a random number is generated for every value of concentration, hydraulic conductivity, and hydraulic gradient entered by the user. This set of random inputs is then used to create and interpolate the respective grids and mass flux calculated from those grids. Repeating this procedure a large number times yields a probability distribution of the mass flux from which statistical characteristics such as mean, percentile, and

variance can be obtained. However, the standard Monte Carlo technique tends to be time intensive because of the large number of iterations requires.

Latin hypercube sampling is a type of stratified Monte Carlo sampling. It can be viewed as a method for controlling the upper and lower ends of the distributions used in the analysis such that all portions of the distribution are well represented (U.S. EPA, 1997; Iman and Helton, 1988; Gwo *et al.*, 1996; Helton and Davis, 2002). In LHS, the given range of each variable in $X_1, \dots, X_n$ is divided into j number of equal non-overlapping probability intervals. A random number with respect to the probability density is then obtained for X_i for each j interval. The j values of X_1 that are obtained are then randomly paired with the j values obtained for X_2 and so on until all the j values in X_n are paired (Iman and Helton, 1988). LHS ensures that a minimal number of probability intervals are required to represent the full range of the distribution (Bergin *et al.*, 1999). Additionally, LHS requires fewer simulations than simple random sampling to achieve the same level of precision (U.S. EPA, 1997; Helton and Davis, 2002), hence a fraction of the time involved with simple random sampling.

LHS sampling was retained as the methodology of choice in the Mass Flux Toolkit for computational efficiency.

Impact of Mass Flux

The Mass Flux Toolkit software has models for determining the impact of mass flux for plumes approaching a stream or supply well.

Receptor Impact Worksheet – Wells

The Toolkit determines the maximum concentration in water extracted from a supply well using the relationship described by Einarson and Mackay (2001a):

$$C_{sw} = M_d / Q_{sw}$$

where:

C_{sw} = the maximum concentration of a contaminant in water extracted from a supply well (mass/volume)

Q_{sw} = is the pumping rate from the supply well (volume/time), and

M_d = the total mass flux or mass discharge of the contaminant from the well (mass/time), which can be predicted before the plume reaches the well using the entire mass flux through upgradient transects.

Additionally, the Toolkit calculates the capture zone of the supply well using the relationship described by Javandel and Tsang (1986), directing the user to alter the transect dimensions if the transect does not encompass the capture zone, thus ensuring accuracy in the model.

Receptor Impact Worksheet – Streams

The Toolkit applies the dilution calculation used for water supply wells to plumes that are discharging to streams.

Guidelines for selecting key input parameters for the model are outlined in [Receptor Impact Data Entry](#). For help on results see [Impact of Receptor – Wells Results](#) and [Impact of Receptor – Streams Results](#).

MASS FLUX TRANSECT CALCULATOR

MASS FLUX TRANSECT CALCULATOR

[MAIN SCREEN](#)

[INPUT DATA AND GRID](#)

[GRID COMPLETION](#)

[MASS FLUX RESULTS](#)

[FINAL CONCENTRATION GRID](#)

[MASS FLUX SUMMARYUNCERTAINTY ANALYSIS](#)

Three important considerations regarding data input are:

- 1) To see the example data set in the input screen of the software, click on the *Paste Example* button on the lower right portion of the input screen.
- 2) Because the Mass Flux Toolkit is based on the Excel spreadsheet, you have to click outside of the cell where you just entered data or hit *Return* before any of the buttons will work. Additionally, **REMOVING** rows or columns from input screens may cause the program to crash.
- 3) Parameters used in the model are to be entered directly into the white cells.

NOTE: Although literature values are provided, it is strongly recommended that the user employ measured hydrogeological and source characteristic values whenever possible. If literature values are used and there is uncertainty in the value chosen, sensitivity analyses should be conducted to determine the effects of the uncertainty on model predictions.

Mass Flux Transect Calculator Data Entry

PARAMETER	UNIT SYSTEM
Description	Unit system to perform mass flux calculations in.
How to Enter Data	Choose the appropriate radio button.

PARAMETER	CONCENTRATION UNITS
Units	mg/L or ug/L
Description	Concentration measurement units.
How to Enter Data	Choose from drop down list.

PARAMETER	ELEVATION UNITS
Units	Below ground surface (bgs) or Mean Sea Level (MSL)
Description	Elevation measurement units.
How to Enter Data	Choose from drop down list. If MSL is selected then a value for the Ground Surface Elevation must be entered.

PARAMETER	CONTINUE INPUT OF TRANSECT DATA
Description	Proceeds to the next step in entering data for mass flux calculations.

PARAMETER	RETURN TO MAIN SCREEN
Description	Returns to the Mass Flux Toolkit Main Screen.

PARAMETER	NEW SITE
Description	Clears ALL data in the Toolkit memory banks. Use this button to start a new project.

PARAMETER	PASTE EXAMPLE
Description	Clears ALL data in the Toolkit memory banks and pastes an example dataset. The example dataset used in the Toolkit is obtained from the API's "Groundwater Remediation Strategies Tool" (Newell <i>et al.</i> , 2003).

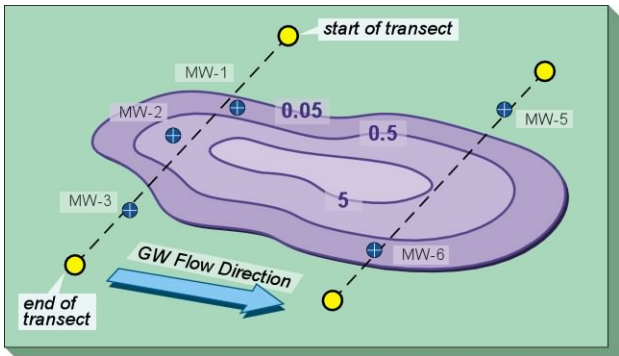
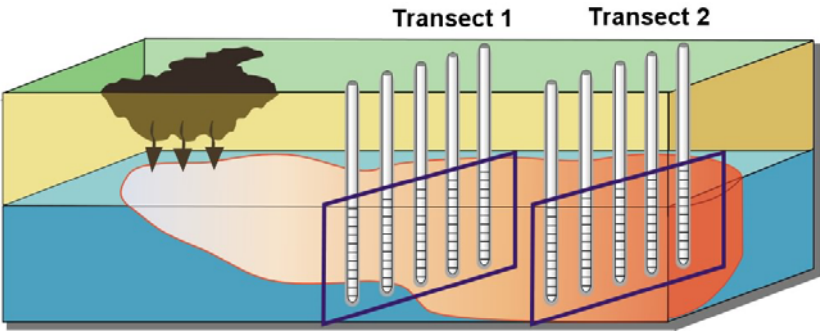
PARAMETER	LOAD FILE
Description	Loads data files saved through the Toolkit. DO NOT EDIT ANY TOOLKIT FILES. Editing files may cause the Toolkit to crash.

TRANSECT MAIN SCREEN DATA ENTRY

PARAMETER	SAVE FILE
Description	Saves all Transect and Receptor Impact data entered into the Toolkit. DO NOT ADD ANY EXTENSTIONS TO FILE NAME WHEN SAVING.

PARAMETER	PRINT
Description	Prints the data shown on the screen on the default printer. To print on a different printer, select the printer in the "Print" options in Excel and then press the "Print" button in the Toolkit.

Input Data and Grid: *Choose Transect*

PARAMETER	TRANSECT
Description	The plane perpendicular to groundwater flow representing vertical distribution of plume concentration. To characterize mass flux, transects should be located at points where sufficient data are available to define affected groundwater concentrations and specific discharge. For two-dimensional data (i.e., from single-screen monitoring wells), the transect will represent a line extending across the full width of the plume, perpendicular to the direction of groundwater. For uniform flow fields, this transect will be a straight line, but, for converging or diverging flowlines, the transect will be curvilinear in shape. For three-dimensional data (i.e., from multilevel monitoring wells), the transect line will represent a vertical plane through the groundwater plume, positioned perpendicular to groundwater flow.  Transects through 2-D Plume.  Transects through 3-D Plume Delineation.
How to Enter Data	Choose the appropriate transect from the drop down list. Data for up to five different plume transects can be entered into the Toolkit.

Input Data and Grid: *Choose Time Period*

PARAMETER	TIME PERIOD
Description	Data collection time period.

INPUT DATA AND GRID

How to Enter Data	Choose the appropriate time period from the drop down list. At least one concentration value must be entered for the data to be saved. Data for up to five different time periods can be entered into the Toolkit When entering data for an additional time period for a particular transect, the user has the option of automatically keeping previously entered data (such as the well name, sampling interval, etc). Select the parameter information to keep from the "Data to Keep" options window.
-------------------	--

Input Data and Grid: *Enter Transect Data*

PARAMETER	DISTANCE OF TRANSECT FROM SOURCE
Units	ft (or m)
Description	Distance of the plume transect of interest from the source. The source zone is defined as the zone that includes the affected soils in both the vadose and smear zones. This value is only used in a summary plot that shows mass flux vs. distance from the plume (maximum of five different transects)
How to Enter Data	Enter directly.

PARAMETER	DARCY VELOCITY
Units	cm/sec, ft(or m)/day, ft(or m)/yr
Description	Groundwater Darcy velocity through the <i>transect</i> of interest. To characterize the specific discharge across each plume transect, representative measurements of the Darcy velocity should be obtained at one or more locations, using appropriate slug or pumping test methods.
Typical Values	0.2 - 200 ft/yr (Newell <i>et al.</i> , 1996)
Source of Data	Calculated by multiplying hydraulic conductivity by hydraulic gradient ($V_d = K * i$). Use of actual site data for hydraulic conductivity and hydraulic gradient parameters is strongly recommended.
How to Enter Data	1) Select appropriate radio button, 2) Select units, and 3) Enter directly: a) As a uniform value for the entire transect, or b) Individually at each sampling depth for each monitoring point.

PARAMETER	HYDRAULIC CONDUCTIVITY
Units	cm/sec, ft(or m)/day, ft(or m)/yr
Description	Measure of the permeability of the saturated porous medium. To characterize the specific discharge across each plume transect, representative measurements are required for both the hydraulic flow gradient and the hydraulic conductivity of the flow system. The groundwater

INPUT DATA AND GRID

	flow direction and hydraulic gradient for each segment of a transect line can be determined from a potentiometric surface contour map based on static water level measurements of available sampling points. Representative measurements of the hydraulic conductivity of the groundwater-bearing unit should be obtained at one or more locations, using appropriate slug test or pumping test methods (Newell <i>et al.</i> , 2003).
Typical Values	Clays: $<1 \times 10^{-6}$ cm/s Silts: 1×10^{-6} - 1×10^{-3} cm/s Silty sands: 1×10^{-5} - 1×10^{-1} cm/s Clean sands: 1×10^{-3} - 1 cm/s Gravels: > 1 cm/s (Newell <i>et al.</i>, 1996)
Source of Data	Pump tests or slug tests at the site. It is strongly recommended that actual site data be used for all mass flux studies.
How to Enter Data	1) Select appropriate radio button, 2) Select units, and 3) Enter directly: a) As a uniform value for the entire transect, or b) Individually at each sampling depth for each monitoring point.

PARAMETER	HYDRAULIC GRADIENT
Units	ft/ft (or m/m)
Description	The slope of the potentiometric surface. In unconfined aquifers, this is equivalent to the slope of the water table.
Typical Values	0.0001- 0.1 ft/ft
Source of Data	Calculated by constructing potentiometric surface maps using static water level data from monitoring wells and estimating the slope of the potentiometric surface.
How to Enter Data	Enter directly: a) As a uniform value for the entire transect, or b) Individually at each sampling depth for each monitoring point.

PARAMETER	SAMPLING INTERVAL
Units	ft bgs, ft MSL, m bgs, or m MSL
Description	The vertical interval from which concentration data is obtained. This option is used when most or all of the monitoring points have defined screen intervals. The sampling interval is the screening interval of the monitoring well in units of distance below ground surface or elevation in MSL. (For direct push-type samples, used the <i>Mid Point of Sampling Interval</i> option). (Note: if you have mixtures of monitoring wells (with screened intervals) or monitoring points (just a single sampling point depth), you need to have all points be represented with either the <i>Sampling Interval</i> method or the <i>Mid</i>

INPUT DATA AND GRID

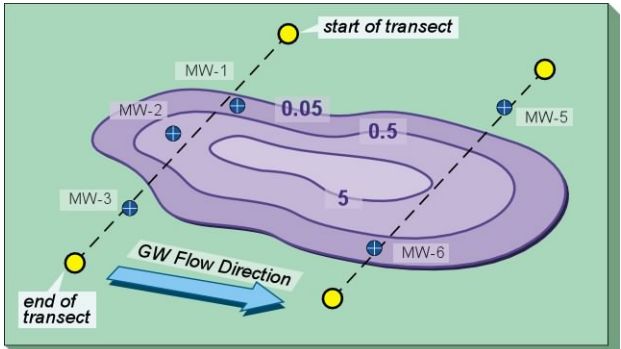
	<i>Point of Sampling Interval</i> method). For each selected plume transect, sufficient groundwater sampling points must be available to define i) the full width and thickness of the plume and ii) the distribution of contaminant concentrations within the plume. Either single-level or multilevel groundwater monitoring points may be used for this purpose. Multilevel monitoring points can provide a more detailed three-dimensional characterization of contaminant concentrations in groundwater. However, single-level groundwater monitoring networks, while less accurate than multi-level networks, can still provide sufficient accuracy to support a mass flux analysis at many sites (Newell <i>et al.</i>, 2003).
Typical Values	3 - 20 ft
Source of Data	Well installation logs.
How to Enter Data	1) Select appropriate radio button, and 2) Enter directly.

PARAMETER	MID POINT OF SAMPLING INTERVAL
Units	ft bgs (or m bgs), ft MSL (or m MSL)
Description	The mid point of the interval from which concentration data is obtained. This option is used when you have a direct push type sample with a very small screen that can be considered a single value. Typically this is the mid point of screening interval of the monitoring point. For monitoring wells with screened intervals, you can use the mid- point of the screened interval, or use the <i>Sampling Interval</i> method. (Note: if you have mixtures of monitoring wells (with screened intervals) or monitoring points (just a single sampling point depth), you need to have all points be represented with either the <i>Sampling Interval</i> method or the <i>Mid Point of Sampling Interval</i> method). For each selected plume transect, sufficient groundwater sampling points must be available to define i) the full width and thickness of the plume and ii) the distribution of contaminant concentrations within the plume. Either single-level or multilevel groundwater monitoring points may be used for this purpose. Multilevel monitoring points can provide a more detailed three-dimensional characterization of contaminant concentrations in groundwater. However, single-level groundwater monitoring networks, while less accurate than multi-level networks, can still provide sufficient accuracy to support a mass flux analysis at many sites (Newell <i>et al.</i>, 2003).
Source of Data	Well installation logs.
How to Enter Data	1) Select appropriate radio button, and 2) Enter directly. The maximum number of lines of data that can be entered is 250.

PARAMETER	MONITORING POINT
Description	For each selected plume transect, sufficient groundwater sampling points must be available to define i) the full width and thickness of the plume and ii) the distribution of contaminant concentrations within the plume. Either single-level or multilevel groundwater monitoring points may be used for this

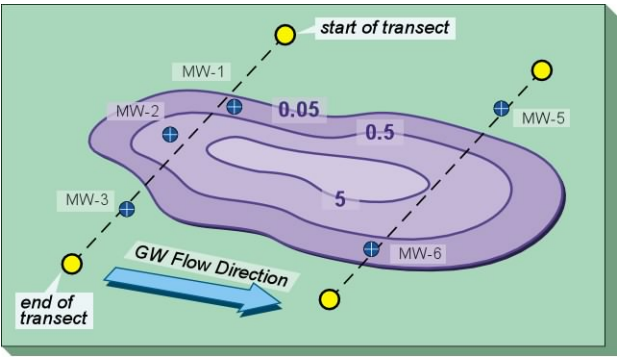
INPUT DATA AND GRID

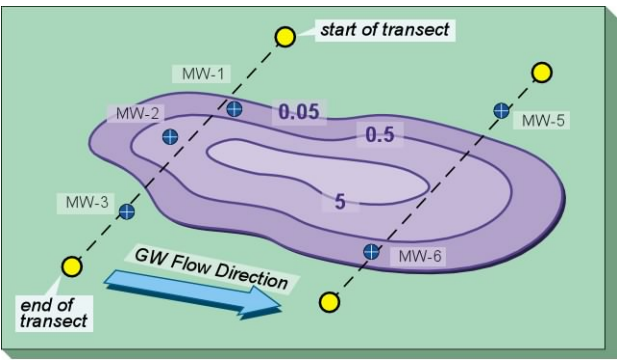
	purpose. Multilevel monitoring points can provide a more detailed three-dimensional characterization of contaminant concentrations in groundwater. However, single-level groundwater monitoring networks, while less accurate than multi-level networks, can still provide sufficient accuracy to support a mass flux analysis at many sites. (NOTE: an alternative method is to use the concentrations from contour lines as measurement points. The locations where the transect intersects contour lines from plume maps can be used to construct flow areas for the mass flux calculations) (Newell <i>et al.</i>, 2003).
Source of Data	Plume maps.
How to Enter Data	Enter directly. The maximum number of monitoring points that can be entered is 100, while the maximum number of lines of data that can be entered is 250.

PARAMETER	START OF TRANSECT
Units	ft (or m)
Description	The Mass Flux Toolkit calculates mass flux based on a two-dimensional grid obtained by dividing the transect into subareas. For this purpose, an edge of the transect is defined as the origin and the locations of all monitoring points based on that origin. The start of the transect is automatically designated as the origin, the user must provide a distance representing the total length of the transect.  Transects through 2-D Plume.

PARAMETER	END OF TRANSECT
Units	ft (or m)
Description	Total length of transect. The Mass Flux Toolkit calculates mass flux based on a two-dimensional grid obtained by dividing the transect into subareas. For this purpose, an edge of the transect is defined as the origin and the locations of all monitoring points based on that origin. The start of the transect is automatically designated as the origin, the user must provide a distance representing the total length of the transect.

INPUT DATA AND GRID

	 Transects through 2-D Plume.
Typical Values	10-500 ft
Source of Data	To determine a transect, draw a line perpendicular to the direction of groundwater flow in the plume area. Define either the left or the right edge of the transect as the origin. Calculate the distances of all monitoring points defining the transect from that origin.
How to Enter Data	Enter directly. Note that the 'End of Transect' distance must be greater than the distance of the farthest well from the start of the transect.

PARAMETER	DISTANCE OF MONITORING POINT FROM START OF TRANSECT
Units	ft (or m)
Description	Distance of monitoring point from start of transect. The Mass Flux Toolkit calculates mass flux based on a two-dimensional grid obtained by dividing the transect into subareas. For this purpose, an edge of the transect is defined as the origin and the locations of all monitoring points based on that origin. The start of the transect is automatically designated as the origin, the user must provide a distance representing the total length of the transect.  Transects through 2-D Plume.
Typical Values	10-500 ft
Source of Data	To determine a transect, draw a line perpendicular to the direction of groundwater flow in the plume area. Define either the left or the right edge of the transect as the origin. Calculate the distances of all monitoring points defining the transect from that origin.

INPUT DATA AND GRID

How to Enter Data	Enter directly. Note that the distance of the first well from the "Start of Transect" must be > 0 while the 'End of Transect' must be greater than the distance of the farthest well from the start of the transect.
-------------------	--

PARAMETER	PLUME TOP
Units	ft bgs (or m bgs), ft MSL (or m MSL)
Description	Top of contaminant plume. For each selected plume transect, sufficient groundwater sampling points must be available to define the thickness of the plume.
Typical Values	5-500 ft bgs
Source of Data	Multilevel groundwater monitoring points.
How to Enter Data	Enter directly. The maximum number of lines of data that can be entered is 250.

PARAMETER	PLUME BOTTOM
Units	ft bgs (or m bgs), ft MSL (or m MSL)
Description	Bottom of contaminant plume. For each selected plume transect, sufficient groundwater sampling points must be available to define the thickness of the plume.
Typical Values	5-500 ft bgs
Source of Data	Multilevel groundwater monitoring points.
How to Enter Data	Enter directly. The maximum number of lines of data that can be entered is 250.

PARAMETER	CONCENTRATION
Units	mg/L or ug/L
Description	Aqueous phase concentration of constituents in the transect of interest. For each selected plume transect, sufficient groundwater sampling points must be available to define i) the full width and thickness of the plume and ii) the distribution of contaminant concentrations within the plume. Either single-level or multilevel groundwater monitoring points may be used for this purpose. Multilevel monitoring points can provide a more detailed three-dimensional characterization of contaminant concentrations in groundwater. However, single-level groundwater monitoring networks, while less accurate than multi-level networks, can still provide sufficient accuracy to support a mass flux analysis at many sites. (NOTE: an alternative method is to use the concentrations from contour lines as measurement points. The locations where the transect intersects contour lines from plume maps can be used to construct flow areas for the mass flux calculations) (Newell <i>et al.</i>, 2003).

INPUT DATA AND GRID

	NOTE: The Toolkit assumes the concentrations at the start and end of the transect are zero.
Typical Values	0.0001 - 500 mg/L
Source of Data	Monitoring well data.
How to Enter Data	1) Enter name of constituent. 2) Enter concentration values. The maximum number of lines of data that can be entered is 250.

PARAMETER	CHOOSE GRID
Description	Subareas the transect plane is divided into for mass flux calculations. The width of the grid cells is obtained from the distance between monitoring points. The thickness of the cells is based on the plume width and length of sampling intervals. The columns in the default grid extend half way on either side between adjacent monitoring points. The width of the columns and thickness of the cells can be decreased by refining the grid.
Typical Values	1 x 1 to 3 x 3 (for 10 or less monitoring points per transect)
Source of Data	.Monitoring well data and plume maps.
How to Enter Data	1. The default refinement is 1 by 1. To refine the default grid, enter the factors to divide the cell thickness and width with. 2. Enter directly. NOTE: Although the maximum grid refinement is 10 for rows and 100/total number of sampling points for columns (resulting in a maximum grid of 100 rows and 100 columns), the greater the grid refinement the greater the computational time. For 10 monitoring points or less, a maximum grid refinement of 3 x 3 is recommended for most computers.

INPUT DATA AND GRID

PARAMETER	SELECT CONSTITUENT OF INTEREST
Description	Select the constituent to use in the mass flux calculations.
How to Enter Data	Select radio button.

PARAMETER	CONTINUE DATA INPUT
Description	Creates the concentration grid to be used in the mass flux calculations.

PARAMETER	EXPORT MW DATA
Description	The Mass Flux Toolkit allows the monitoring well data entered on the Input Data and Grid screen to be exported into a text file for use in other programs. The Toolkit exports data one transect and one time period at a time into tab delimited text file.

Import/Export File Format

Transect Number	Time Period Number													
(enter value)	(enter value)													
System Units	Elevation Units	Ground Surface Elevation												
1 = English 2 = SI	1 = bgs 2 = MSL	(enter value if MSL)												
Concentration Units	Darcy Or Conductivity?	Darcy/ Conductivity Units												
1 = mg/L 2 = ug/L	1 = Darcy 2 = Conductivity	1 = cm/sec 2 = ft/d 3 = ft/yr												
Uniform Darcy/ Conductivity?	Uniform Darcy/ Conductivity Value	Uniform Gradient?	Uniform Gradient Value											
1 = yes 2 = no	(enter value if uniform)	1 = yes 2 = no (leave blank if Darcy)	(enter value if uniform or leave blank if Darcy)											
Distance From Source	Sampling Interval or Midpoint?	End of Transect												
(enter value)	1 = Interval 2 = Midpoint	(enter value)												
Name	Distance from Start of Transect	Sampling Interval Top	Sampling Interval Bottom	Midpoint of Sampling Interval	Plume Top	Plume Bottom	Leave Column Blank	Leave Column Blank	Darcy Velocity	Hydraulic Conductivity	Hydraulic Gradient	COC_A	COC_B	

Sample File

4	1													
1	1													
1	2	3												
1	0.032	1	0.002											
884 3	1	60												
Name	Distance	IntervalTop	IntervalBottom		PlumeTop	PlumeBot				Conductivity	Gradient	COC_A		
MW-2	10	6	10		5	20				0.082	0.002	1.2		
MW-2	10	10	15		5	20				0.082	0.002	0.05		
MW-2	10	15	20		5	20				0.082	0.002	0.05		
TRZ-8	35	6	10		5	20				0.082	0.002	2.67		
TRZ-8	35	10	15		5	20				0.082	0.002	1.42		
TRZ-8	35	15	20		5	20				0.082	0.002	0.05		
TRZ-19	57.5	6	10		5	20				0.082	0.002	1.13		
TRZ-19	57.5	10	15		5	20				0.082	0.002	0.68		
TRZ-19	57.5	15	20		5	20				0.082	0.002	0.05		

PARAMETER	IMPORT MW DATA
Description	The Mass Flux Toolkit allows monitoring well data to be imported from a tab-delimited text file. The Toolkit imports data one transect and one time period

INPUT DATA AND GRID

	at a time.
Imported File Format	See Exported File Format above.
How to Enter Data	Enter values in cells where data is available. Leave cells with no data blank.

PARAMETER	BACK TO TRANSECT MAIN
Description	Returns to the Mass Flux Transect Calculator main screen.

PARAMETER	CLEAR SCREEN
Description	Clears the data in the Toolkit memory banks for the selected transect and time period . Use this button to clear the screen.

PARAMETER	PASTE EXAMPLE
Description	Clears ALL data in the Toolkit memory banks and pastes an example dataset. The example dataset used in the Toolkit is obtained from the American Petroleum Institute's (API) "Groundwater Remediation Strategies Tool" (Newell <i>et al.</i> , 2003).

PARAMETER	RESTORE TABLE FORMATTING
Description	If you pasted data into the table portion of the screen from another excel sheet, then this button will restore the Toolkit formatting to the table.

PARAMETER	SEE SAVED GRIDS
Description	Proceeds to the Final Concentration Grid screen if any mass flux has been calculated previously.

PARAMETER	PRINT
Description	Prints the data shown on the screen on the default printer. To print on a different printer, select the printer in the "Print" options in Excel and then press the "Print" button.

PARAMETER	SELECT DATA TO KEEP FROM PREVIOUS TIME PERIOD
Description	Gives the user the option of keeping data already entered for a Transect Time Period for the next Time Period. This user can select to copy over all the listed parameters, none of the parameters, or customize the selection of parameters to copy from the preceding Time Period.

Method for Interpolating Grid

PARAMETER	CHOOSE A METHOD FOR INTERPOLATING GRID
Description	The user specifies which of three averaging methods will be used to interpolate the concentration, conductivity/Darcy velocity, and gradient grids: user-defined, nearest neighbor, or interpolation (linear interpolation or log transformation). Interpolated concentration data can be edited by directly selecting the desired cell in the grid. User Defined When the user-defined method is chosen, the user must interpolate the concentrations manually. Nearest Neighbor When the nearest neighbor option is chosen, the model assigns values to each cell based on the closest input data point. Linear Interpolation When the linear interpolation option is chosen, the grid is first interpolated vertically and then horizontally. The user has to further select whether to use a) linear interpolation or b) log transformation to interpolate the horizontal cells in the grid. Log Transformation Interpolation Under this option, the natural logarithms of the values are obtained, interpolations performed, and the interpolated data re transformed. When the log transformation option is chosen, the grid is first interpolated vertically then horizontally. The user has to further select whether to use a) linear interpolation or b) log transformation to interpolate the horizontal cells in the grid. NOTE: The Toolkit also allows the grid to be interpolated outside of the Toolkit. For this purpose, a) the “User Defined” option should be chosen, b) the grid “exported” using the <i>Export Grid</i> function in the Toolkit, c) interpolated by user outside the Toolkit, and d) imported back into the Toolkit.
How to Enter Data	1. Select radio button (Step 9). 2. If the “interpolation” option is selected then a. Select the interpolation scheme for vertical interpolation of the grid (Step 9A). b. If desired, edit interpolated values. c. Select the interpolation scheme for horizontal interpolation of the grid (Step 10). 3. Interpolated data can be edited by directly selecting the desired cell in the grid.

Grid Completion: *Interpolate Concentration, Conductivity, and Gradient*

Before total mass flux can be calculated, the following grids must be interpolated:

1. Concentration
2. Darcy Velocity/Hydraulic Conductivity
3. Hydraulic Gradient (if necessary)

To get back to the previously calculated mass flux grid do the following:

- a. Press '**Back to Data Input**' button
- b. Press '**See Conc/Flux Grids**' button
- c. Press '**View Mass Flux Result**' button

PARAMETER	INTERPOLATE HORIZONTALLY
Description	When the linear or log transformation interpolation option is chosen in Step 9 , the user has to select whether to use a) linear interpolation or b) log transformation to interpolate the horizontal rows of the grid.
How to Enter Data	1. Select the interpolation scheme for horizontal interpolation of the grid (Step 10). 2. Interpolated data can be edited by directly selecting the desired cell in the grid.

PARAMETER	EXPORT GRID
Description	The Mass Flux Toolkit allows the exporting of the concentration/conductivity/gradient grids into a text file for external interpolation. Note that the Toolkit only exports the grid currently shown on the screen.

PARAMETER	IMPORT GRID
Description	The Mass Flux Toolkit allows the exporting/importing of the concentration/conductivity/gradient grids into a text file for external interpolation. NOTE: Any externally interpolated grid being imported into the Toolkit MUST have the same number of rows and columns as the Toolkit grid. Additionally, uncertainty analysis is not available for imported grids.

PARAMETER	CALCULATE MASS FLUX
Description	The total contaminant mass flux across the transect is calculated as follows: $w = \sum_{i=1}^{i=n} C_i q_i A_i CF$ where:

GRID COMPLETION

	w = total mass flux from source zone (g/day) (also called mass discharge) C_i = concentration of constituent at flow area in transect (mg/L) q_i = specific discharge (also called Darcy velocity) through flow area associated with an individual constituent measurement i (cm/sec). q_i can be calculated using $q_i = K \cdot i$ where: K = hydraulic conductivity (cm/sec) i = hydraulic gradient (cm/cm) A_i = Flow area associated with an individual constituent measurement (ft²) CF = conversion factor = 80.3 (ft/cm)/(sec/day)(L/ft³)(g/mg)
--	--

PARAMETER	BACK TO DATA INPUT
Description	Returns to the Input Data and Grid screen.

PARAMETER	BACK TO CONC GRID
Description	Returns to the Grid Completion: Concentration screen.

PARAMETER	BACK TO K/DARCY GRID
Description	Returns to the Grid Completion: Hydraulic Conductivity/Darcy Velocity screen.

PARAMETER	PRINT
Description	Prints the data shown on the screen on the default printer. To print on a different printer, select the printer in the "Print" options in Excel and then press the "Print" button.

Mass Flux Results

PARAMETER	TOTAL MASS FLUX
Description	The total contaminant mass flux across the transect in g/day and kg/yr.

PARAMETER	MASS FLUX SUMMARY
Description	Takes the user to Mass Flux Summary screen.

PARAMETER	RUN/VIEW UNCERTAINTY ANALYSIS
Description	Uncertainty in mass flux estimates is a key issue in using mass flux as a metric. The Toolkit provides two options for analyzing uncertainty in the total mass flux estimates derived from the transect method. One option (Simple Uncertainty Analysis) provides a tool for estimating the contribution of each individual observation to the total mass flux. If a single monitoring point represents a high percentage of the total mass flux, then the uncertainty in the calculation is high and additional monitoring points should be added to reduce the uncertainty. The second option (Advanced Uncertainty Analysis) utilizes a Monte Carlo type approach to analyze uncertainty in the actual concentration, hydraulic conductivity, and gradient measurements. With this tool, groundwater practitioners can estimate the accuracy of the hydrologic measurements that are being used for the mass flux calculation.

PARAMETER	SELECT TRANSECT TO VIEW
Description	Select a different transect to view. This option allows the user to see previously calculated flux grids.

PARAMETER	SELECT TIME PERIOD TO VIEW
Description	Select a different time period to view. This option allows the user to see previously calculated flux grids.

PARAMETER	VIEW CONCENTRATION GRID
Description	Takes the user to the Final Concentration Grid screen. The concentration values in this grid cannot be edited. To edit concentration values return to the "Grid Completion" screen.

PARAMETER	BACK TO DATA GRID
Description	Returns to the Input Data and Grid screen.

MASS FLUX RESULTS

PARAMETER	PRINT
Description	Prints the data shown on the screen on the default printer. To print on a different printer, select the printer in the "Print" options in Excel and then press the "Print" button.

Final Concentration Grid

PARAMETER	SELECT TRANSECT TO VIEW
Description	Select a different transect to view. This option allows the user to see previous grids.

PARAMETER	SELECT TIME PERIOD TO VIEW
Description	Select a different time period to view. This option allows the user to see previous grids.

PARAMETER	MASS FLUX SUMMARY
Description	Takes the user to Mass Flux Summary screen.

PARAMETER	VIEW MASS FLUX RESULTS
Description	Takes the user to the Mass Flux Results screen.

PARAMETER	VIEW FINAL CONC GRID
Description	Shows the user the Final Concentration grid. This screen is for viewing purposes only and data cannot be edited. To edit grid data use the 'Back to Data Grid' button; to edit monitoring well input data use the 'Back to Data Input' button.

PARAMETER	VIEW FINAL K/DARCY GRID
Description	Shows the user the Final Hydraulic Conductivity or Darcy Velocity grid. This screen is for viewing purposes only and data cannot be edited. To edit grid data use the 'Back to Data Grid' button; to edit monitoring well input data use the 'Back to Data Input' button.

PARAMETER	VIEW FINAL I GRID
Description	Shows the user the Final Hydraulic Conductivity grid. This screen is for viewing purposes only and data cannot be edited. To edit grid data use the 'Back to Data Grid' button; to edit monitoring well input data use the 'Back to Data Input' button.

PARAMETER	PRINT
Description	Prints the data shown on the screen on the default printer. To print on a different printer, select the printer in the "Print" options in Excel and then press the "Print" button.

Mass Flux Summary

PARAMETER	SUMMARY GRAPH
Description	The summary graph plots mass flux vs. distance to show the effect of remediation/impact of natural attenuation processes. A maximum of two types of error bars are shown on the graph. The first one (interpolation error bar) represents the minimum and maximum mass fluxes calculated using all the three available interpolation schemes in the Toolkit. The other set of error bars (input interpolation) represent the 15th and 85th percentiles from the Advanced Uncertainty analysis (for the particular interpolation scheme(s) chosen by the user to interpolate concentration, conductivity, and gradient). This set of error bars will only be shown when an Advanced Uncertainty analysis is performed by the user.

PARAMETER	RETURN TO TOOLKIT MAIN SCREEN
Description	Returns to the Mass Flux Toolkit main screen.

PARAMETER	RETURN TO TRANSECT MAIN SCREEN
Description	Returns to the main screen of the Mass Flux Transect Calculator.

PARAMETER	VIEW MASS FLUX RESULTS
Description	Returns to the Mass Flux Results screen.

PARAMETER	VIEW CONC GRID
Description	Returns to the Final Concentration Grid screen. The concentration values in this grid cannot be edited. To edit concentration values return to the "Grid Completion" screen.

PARAMETER	PRINT
Description	Prints the data shown on the screen on the default printer. To print on a different printer, select the printer in the "Print" options in Excel and then press the "Print" button.

Uncertainty Analysis: Perform Uncertainty Analysis

Uncertainty in mass flux estimates is a key issue in using mass flux as a metric. The Toolkit provides two options for analyzing Type 1 uncertainty in the total mass flux estimates derived from the transect method.

One option (Simple Uncertainty Analysis) provides a tool for estimating the contribution of each individual observation to the total mass flux. If a single monitoring point represents a high percentage of the total mass flux, then the uncertainty in the calculation is high and additional monitoring points should be added to reduce the uncertainty.

The second option (Advanced Uncertainty Analysis) utilizes the Monte Carlo approach to analyze uncertainty in the actual concentration, hydraulic conductivity, and gradient measurements. With this tool, groundwater practitioners can estimate the accuracy of the hydrologic measurements that are being used for the mass flux calculation.

PARAMETER	SIMPLE UNCERTAINTY ANALYSIS (EVALUATE UNCERTAINTY IN INTERPOLATION SCHEME)
Description	This module applies crossvalidation to evaluate the uncertainty in the interpolation scheme. Crossvalidation is a method of removing one observation at a time, estimating a value for the removed observation using the remaining observations, and calculating the output (Olea, 1999). The removed value is then replaced and the next observation removed. This process is continued until all the observations have been removed one at a time. The Toolkit removes each observed value of concentration, hydraulic conductivity, and gradient one at a time during crossvalidation, creates and interpolates the grid using the same options chosen in the 'Grid Completion' screen, and calculates mass flux.
How to Enter Data	Press 'Evaluate Uncertainty in Interpolation Scheme'. NOTE: The default interpolation scheme that the Toolkit uses is the nearest neighbor interpolation.. Uncertainty analysis assumes that the Toolkit interpolated concentrations have not been manually edited. Uncertainty analysis is not available for manually created grids.

PARAMETER	ADVANCED UNCERTAINTY ANALYSIS (EVALUATE HOW UNCERTAINTY IN INPUT DATA AFFECTS TOTAL MASS FLUX)
Description	This module uses Latin hypercube sampling (LHS), a modified Monte Carlo approach, to analyze uncertainty in the actual concentration, hydraulic conductivity, and gradient measurements. In the Monte Carlo type approach, a random number is generated for every value of concentration, hydraulic conductivity, and hydraulic gradient entered by the user. This set of random inputs is then used to create and interpolate the respective grids and mass flux calculated from those grids. Repeating this procedure a large number times yields a probability distribution of the mass flux from which statistical characteristics such as mean, percentile, and

UNCERTAINTY ANALYSIS

	variance can be obtained. The Mass Flux Toolkit performs 10 LHS iterations of 20 equal probability intervals (See Appendix 1 for details on Latin hypercube sampling).
How to Enter Data	1) Specify global parameters for the concentration, Darcy/Conductivity, and gradient. The Toolkit assumes that the values entered in the Input screen are the mean values: a. Choose a probability distribution for each parameter (see Appendix A of the User's Manual for details on probability distributions). b. For the normal distribution, specify the standard deviation as a percent of the mean. For lognormal distributions, specify the error factor (EF) (the ratio of the 95th percentile to the median of the lognormal data or the ratio of the median to the 5th percentile) (NOTE: the error factor MUST be greater than one). For uniform distribution, specify the lower and upper limits as percentages of the mean. 2) If desired, Monte Carlo parameters for each individual value of concentration, Darcy/Conductivity, and gradient can be specified using the 'Edit Individual Values Manually' option. 3) Perform Input Uncertainty Analysis. NOTE: Uncertainty analysis is performed on the transect and time period selected in the Mass Flux Results screen. Uncertainty analysis assumes that the Toolkit interpolated concentrations have not been manually edited. Uncertainty analysis is not available for manually created grids.

Uncertainty Analysis: Results

PARAMETER	INTERPOLATION ERROR RESULTS (SIMPLE UNCERTAINTY ANALYSIS)
Description	Comparison of the total mass flux calculated using all the observations and the contribution of each removed observation to the total mass flux. If a single monitoring point represents a high percentage of the total mass flux, then the uncertainty in the calculation is high and additional monitoring points should be added to reduce the uncertainty.

PARAMETER	INPUT DATA UNCERTAINTY ANALYSIS RESULTS (ADVANCED UNCERTAINTY ANALYSIS)
Description	Summary statistics (minimum, 25th percentile, mean, 85th percentile, maximum, and variance) on the estimate of uncertainty in the mass flux calculation based on the user's choice of interpolation method and uncertainty in the input variables as defined by their probability distributions, means, variances, and ranges.

UNCERTAINTY ANALYSIS

PARAMETER	BACK TO MASS FLUX RESULTS
Description	Returns to the Mass Flux Results screen.

PARAMETER	BACK TO DATA INPUT
Description	Returns to the Data Input screen.

PARAMETER	PRINT
Description	Prints the data shown on the screen on the default printer. To print on a different printer, select the printer in the "Print" options in Excel and then press the "Print" button.

RECEPTOR IMPACT WORKSHEETS

[Wells](#)
[Streams](#)
[API Strategies Tool](#)

Three important considerations regarding data input are:

- 1) To see the example data set in the input screen of the software, click on the *Paste Example* button on the lower right portion of the input screen.
- 2) Because the Mass Flux Toolkit is based on the Excel spreadsheet, you have to click outside of the cell where you just entered data or hit *Return* before any of the buttons will work. Additionally, **REMOVING** rows or columns from input screens may cause the program to crash.
- 3) Parameters used in the model are to be entered directly into the white cells.

NOTE: These worksheets only work if mass flux has been calculated for at least one transect in the Mass Flux Transect Calculator.

Receptor Impact - Wells: *Input Data*

PARAMETER	SELECT CONSTITUENT OF INTEREST
Description	The constituent to use in the dilution calculations.
How to Enter Data	Select radio button.

PARAMETER	TRANSECT OF INTEREST
Description	The transect to use in the dilution calculations
Source of Data	Plume maps.
How to Enter Data	Select one of the transects for which mass flux has been calculated in the Toolkit.

PARAMETER	TIME PERIOD OF INTEREST
Description	The time period of data entered in the Mass Flux Transect Calculator.
How to Enter Data	Select one of the time periods for which mass flux has been calculated in the Toolkit.

PARAMETER	DISCHARGE RATE OF EACH SUPPLY WELL
Units	gpm, gpd, $\text{ft}^3(\text{m}^3)/\text{min}$, $\text{ft}^3(\text{m}^3)/\text{d}$
Description	Discharge rate of each supply well.
Typical Values	0.1 to 1000 gpm
How to Enter Data	Enter directly.

PARAMETER	NUMBER OF SUPPLY WELLS
Description	Number of supply wells potentially affected by the contaminant plume.
Typical Values	1-5
How to Enter Data	Enter directly.

PARAMETER	AQUIFER THICKNESS
Units	ft (or m)
Description	Estimated thickness of the aquifer containing the supply well and the contaminant plume.
Typical Values	10 to 100 ft

RECEPTOR IMPACT – WELLS DATA INPUT

Source of Data	Typically determined from site boring logs.
How to Enter Data	Enter directly.

Receptor Impact - Wells: Results

PARAMETER	CONSTITUENT CONCENTRATION
Description	The maximum concentration of a contaminant in water extracted from a supply well using the relationship described in Einarson and Mackay (2001): $C_{SW} = M_d/Q_{SW}$ where M_d is the total mass flux or mass discharge of the contaminant from the well, which can be predicted before the plume reaches the well using the entire mass flux through upgradient transects and Q_{SW} is the pumping rate from the supply well.

PARAMETER	CAPTURE ZONE OF SUPPLY WELL
Description	The capture zone of the supply well using the relationship described by Javandel and Tsang (1986).

PARAMETER	DISTANCE OF SUPPLY WELL FROM STAGNATION POINT
Description	The distance of the supply well from the stagnation point using the relationship described by Javandel and Tsang (1986).

Receptor Impact - Streams: *Input Data*

PARAMETER	CONTAMINANT OF INTEREST
Description	The constituent to use in the dilution calculations.
How to Enter Data	Select from radio buttons. .

PARAMETER	TRANSECT OF INTEREST
Description	The transect to use in the dilution calculations
Source of Data	Plume maps.
How to Enter Data	Select one of the transects for which mass flux has been calculated in the Toolkit.

PARAMETER	TIME PERIOD OF INTEREST
Description	The time period of data entered in the Mass Flux Transect Calculator.
How to Enter Data	Select one of the time periods for which mass flux has been calculated in the Toolkit.

PARAMETER	STREAM FLOW RATE
Units	gpm, gpd, $\text{ft}^3(\text{m}^3)/\text{sec}$, $\text{ft}^3(\text{m}^3)/\text{min}$, $\text{ft}^3(\text{m}^3)/\text{d}$
Description	The flowrate of the stream approached by the plume.
Typical Values	0.1 -10 ⁶ cfm
Source of Data	U.S. geological stream gage information
How to Enter Data	Enter directly.

Receptor Impact - Streams: *Results*

PARAMETER	CONSTITUENT CONCENTRATION
Description	The maximum concentration of a contaminant in water extracted from a stream downgradient of plume using the relationship described in Einarson and Mackay (2001): $C_{sw} = M_d/Q_{sw}$ where M_d = the total mass flux or mass discharge of the contaminant from the well, which can be predicted before the plume reaches the stream using the entire mass flux through upgradient transects, and Q_{sw} = the flow rate of the stream.

API STRATEGIES TOOL

The Mass Flux Toolkit provides an electronic version of the American Petroleum Institute's (API) *Groundwater Remediation Strategies Guide* (Newell *et al.*, 2003) to help users apply mass flux to groundwater remediation decision-making. Please refer to the above document ("API Groundwater Remediation Strategies Tool" tab in "Learn About Mass Flux") for help.

CURRENT ESTCP/SERDP MASS FLUX PROJECTS

Several ESTCP and SERDP projects dealing with mass flux are currently ongoing. The following is a list of such projects by lead principal investigator:

- Linda Abriola: Development of Assessment Tools for Evaluation of the Benefits of DNAPL Source Zone Treatment.

This project deals with the development of methodologies for reliable prediction or monitoring of plume development or reduction of organic mass flux under heterogeneous field conditions after the source zone treatment.

Details on this project can be obtained at:

<http://www.serdp.org/research/CU/CU-1293.pdf>

- Kirk Hatfield: Demonstration and Validation of a Water and Solute Flux Measuring Device

This project involves the development of the flux-meter for the quantification of contaminant flux leaving a site. The objective being that risk posed by a site can be better evaluated and remedial efforts made by measuring cumulative flux rather than contaminant concentrations.

Details on this project can be obtained at:

<http://www.estcp.org/projects/cleanup/200114o.cfm>

- Tissa Illangasekare: Mass Transfer from Entrapped DNAPL Sources Undergoing Remediation: Characterization Methods and Prediction Tools.

This project seeks to develop prediction tools and site characterization methods to assist site managers 1) make decisions on managing sites and 2) implement cost and benefit effective remediation technologies. The objective being to understand, quantify, and model the transfer of mass across heterogeneous DNAPL source zones undergoing remediation.

Details on this project can be obtained at:

<http://www.serdp.org/research/cu/cu-1294.pdf>

- Michael Kavanaugh: Diagnostic Tools for Performance Evaluation of Innovative In-Situ Remediation Technologies at Chlorinated Solvent-Contaminated Sites

The objective of this project is to evaluate in-situ remediation technologies at three hydrogeologically different sites by applying mass flux as the metric of overall system performance. Furthermore, the project compares various methods of calculating mass flux.

Details on this project can be obtained at:

<http://www.estcp.org/projects/cleanup/CU-0318.cfm>

- Lynn Wood: Impact of DNAPL Source Zone Treatment: Experimental and Modeling Assessment of Benefits of Partial Source Removal.

This project seeks to develop an understanding of the relationship between source zone remediation and dissolved plume behavior by balancing mass removal with plume attenuation for the purpose of optimizing the remedial process. The objective being the development of cost-effective remediation endpoints based on mass flux.

Details on this project can be obtained at:

<http://www.serdp.org/research/CU/CU-1295.pdf>

REFERENCES

- American Society for Testing and Materials (ASTM), 1998. *Standard Guide for Remediation of Ground Water by Natural Attenuation at Petroleum Release Sites*. Designation: E 1943 – 98. West Conshohocken, Pennsylvania.
- Aziz, C.E., C.J. Newell, J.R. Gonzales, P. Haas, T.P. Clement, and Y-W. Sun, 2000. *BIOCHLOR Version 1.0 User's manual*. U.S. Environmental Protection Agency publication EPA/600/R-00/008.
- Bergin, M. S., G. S. Noblet, K. Petrini, J.R. Dhieux, J.B. Milfold, and R.A. Harley, 1999. "Formal Uncertainty Analysis of a Lagrangian Photochemical Air Pollution Model", Environ. Sci. Technol 33: 1116-1126.
- Bergin, M. S. and J. B. Milford, 2000. "Application of Bayesian Monte Carlo analysis to a Lagrangian photochemical air quality model", Atmospheric Environment 34: 781-792.
- Bockelmann, A., D. Zamfirescu, T. Ptak, P. Grathwohl, and G. Teutsch, 2003. "Quantification of mass fluxes and natural attenuation rates at an industrial site with a limited monitoring network: a case study", Journal of Contaminant Hydrology 60, 97–121.
- Borden, R.C., R.A. Daniel, L.E. LeBrun IV, and C.W. Davis, 1997. "Intrinsic biodegradation of MTBE and BTEX in a gasoline-contaminated aquifer", Water Resources Research v. 38, n. 5, pp. 1105-1115.
- Buscheck, T, 2002. Mass Flux Estimates to Assist Decision-Making: Technical Bulletin. Version 1.0. ChevronTexaco Energy Research and Technology Company, June 2002.
- Connecticut Department of Environmental Protection (CTDEP), 2002. Regulations of Connecticut State Agencies, Title 22A, Environmental Protection, Department of Environmental Protection, Remediation Standard 22a-133K-3.
- Cox, D. C. and P. Baybutt, 1981. "Methods for Uncertainty Analysis: A Comparative Study", Risk Analysis 1(4): 251-258.
- Devlin, J.F, M. McMaster, and J.F Barker, 2002. "Hydrogeologic assessment of in situ natural attenuation in a controlled field experiment", Water Resources Research v. 38, n. 1, 10.1029/2000WR000148.
- Einarson, M.D. and D.M. Mackay, 2001a. "Predicting the Impacts of Groundwater Contamination", Environmental Science and Technology, 35(3): 67A:73A.
- Einarson, M.D. and D. M. Mackay, 2001b. "Supplementary Information to Accompany ES&T Feature Article," February 2001, einarson@ix.netcom.com, d4mackay@uwaterloo.ca.
- Einarson, M.D. and D. M. Mackay, 2002. Presentation to the American Petroleum Institute Soil and Groundwater Technical Task Force, Berkeley, California, October 16, 2002.
- Einarson, M., D. Mackay, N. de Sieyes, L. Jacobson, M. Noske, and L. Justice, 2005. "Evaluation of Point Measurement and Pumping Techniques for Calculating Contaminant Mass Flux at a Non-Steady State MTBE Plume in California", The Abstract Book of the 2005 Ground Water

REFERENCES

- Summit Program, National Ground Water Association, San Antonio, Texas, April 17-20, 2005.
- Fraser, M, R. McLaren, and J. Barker, 2005. "Multilevel Monitoring Wells to Assess Contaminant Mass Discharge: Magnitude of Uncertainties Based on Borden Monitoring Experience", The Abstract Book of the 2005 Ground Water Summit Program, National Ground Water Association, San Antonio, Texas, April 17-20, 2005.
- Gallagher M.N., R.E. Payne, and E.J. Perez, 1995. "Mass Based Corrective Action," Proceedings of the 1995 Petroleum Hydrocarbons and Organic Chemicals in Ground Water: Prevention, Detection, and Restoration Conference and Exposition, Houston, Texas, November 29 - December 1, 1995, pp. 453-465.
- Groundwater Services, Inc., 2002. RBCA Tool Kit. Version 1.3a. Groundwater Services, Inc., Houston, Texas.
- Guilbeault, M.A., B. L. Parker, and J. A. Cherry, 2005. "Mass and Flux Distributions from DNAPL Zones in Sandy Aquifers", Ground Water 43(1): 70-86.
- Gwo, J. P., L. E. Toran, M. D. Morris, and G. V. Wilson, 1996. "Subsurface Stormwater Modeling with Sensitivity Analysis Using a Latin-Hypercube Sampling Technique", Ground Water 34(5): 811-818.
- Javandel, I. and C.F. Tsang, 1986, "Capture-Zone Type Curves: A Tool for Aquifer Cleanup", Groundwater 24(5): 616-625, 1986.
- Hatfield, K., M.D. Annable, S. Kuhn, P.S.C. Rao, and T. Campbell, 2002. "A new method for quantifying contaminant flux at hazardous waste sites", in Groundwater Quality: Natural and Enhanced Restoration of Groundwater Protection, edited by S.F. Thornton and S.E. Oswald, IAHS Publication No. 275, IAHS Press, Oxfordshire, United Kingdom, pp. 25-32.
- Helton, J. C. and F. J. Davis, 2002. "Illustration of Sampling-Based Methods for Uncertainty and Sensitivity Analysis", Risk Analysis 22(3): 591-622.
- Iman, R. L. and J. C. Helton, 1988. "An Investigation of Uncertainty and Sensitivity Analysis Techniques for Computer Models", Risk Analysis 8(1): 71-90.
- Kavanaugh, M.C., S.C. Rao, L. Abriola, J. Cherry, G. Destouni, R. Falta, D. Major, J. Mercer, C. Newell, T. Sale, S. Shoemaker, R. Siegrist, G. Teutsch, and K. Udell, 2003. *The DNAPL Remediation Challenge: Is There a Case for Source Depletion?* National Risk Management Research Laboratory, Ada, Ok, EPA/600/R-03/143, December 2003.
- Newell, C.J., R.K. McLeod, and J.R. Gonzales, 1996. *BIOSCREEN Natural Attenuation Decision Support System*, U.S. Environmental Protection Agency publication EPA/600/R-96/087. Version 1.4 Revisions.
- Newell, C.J., J. A. Connor, and D.L. Rowan, 2003. "Groundwater Remediation Strategies Guide", American Petroleum Institute, Publication Number 4730, Washington, DC, December 2003.
- Nichols, E. M., R. T. Roth, S. Martin, and R. G. Vit Kuhnelt, 2005. "Use of Dissolved Mass Discharge Estimates for Groundwater Resource Protection and Regulatory Compliance", The Abstract Book of the 2005 Ground Water Summit Program, National Ground Water Association, San Antonio, Texas, April 17-20, 2005.
- Olea, R. A., 1999. Geostatistics for Engineers and Earth Scientists, Kluwer Academic Publishers, Boston.

REFERENCES

- Pankow, J. F. and J.A. Cherry, 1996. Dense Chlorinated Solvents and other DNAPLs in Groundwater, Waterloo Press, Waterloo, Ontario.
- Rao, P.S.C., J.W. Jawitz, C.G. Enfield, R.W. Falta, Jr., M.D. Annable, and A.L. Wood, 2002. "Technology Integration for Contaminated Site Remediation: Cleanup Goals & Performance Criteria", in Groundwater Quality: Natural and Enhanced Restoration of Groundwater Protection, edited by S.F. Thornton and S.E. Oswald, IAHS Publication No. 275, IAHS Press, Oxfordshire, United Kingdom, pp. 571-578.
- Rong, Y., R. F. Wang, and R. Chou, 1998. "Monte Carlo Simulation for a Groundwater Mixing Model in Soil Remediation of Tetrachloroethylene", Journal of Soil Contamination 7(1): 87-102.
- SERDP/ESTCP, 2001. Expert Panel Workshop on Research and Development Needs for Cleanup of Chlorinated Solvent Sites, 2001.
- Swiler, L.P. and G.D. Wyss, 2004. A User's Guide to Sandia's Latin Hypercube Sampling Software: LHS Unix Library/Standalone Version, Sandia National Laboratories, Albuquerque, New Mexico.
- Thuma, J., G. Hinshalwood, V. Kremesec, and R. Kolhatkar, 2001. "Application of Ground Water Fate and Transport Models to Evaluate Contaminant Mass Flux and Remedial Options for a MTBE Plume on Long Island, NY." in Proceedings of the 2001 Petroleum Hydrocarbons and Organic Chemicals in Ground Water: Prevention, Detection, and Remediation Conference & Exposition, National Ground Water Association, Houston, Texas, November 14 – 6, 2001.
- U.S. EPA, 1997. *Guiding Principles for Monte Carlo Analysis*, U.S. Environmental Protection Agency, EPA/630/R-97/001, March 1997.
- U.S. Environmental Protection Agency, 1998. *Monitored Natural Attenuation for Ground Water*, Seminar Notes, EPA/625/K-98/001, Washington, DC, September 1998.
- U.S. Environmental Protection Agency (U.S. EPA), 2001. *Monitored Natural Attenuation: USEPA Research Program – An EPA Science Advisory Board Review*. Review by the Environmental Engineering Committee (EEC) of the EPA Science Advisory Board. United States Science Advisory Board (1400A) EPA-SAB-EEC-01-004. Washington DC. www.epa.gov/sab. May 2001.
- Wiedemeier, T.H., H.S. Rifai, C.J. Newell, J.T. Wilson, 1999. Natural Attenuation of Fuels and Chlorinated Solvents in the Subsurface. Wiley, New York, pp. 615.

MASS FLUX TOOLKIT TROUBLESHOOTING TIPS

Minimum System Requirements

The Mass Flux Toolkit model requires a computer system capable of running Microsoft® Excel (2000/XP) for Windows (2000/XP). Operation requires an IBM-compatible PC equipped with a Pentium or later processor running at a minimum of 450 MHz. A minimum of 256 MB of system memory (RAM) is strongly recommended. Computers not meeting these recommendations will experience slow running times and/or problems with memory.

Installation and Start-Up

The software is installed by unzipping the Toolkit model file (MassFluxToolkit.zip) and keeping all the unzipped files in the same folder on your computer hard drive. To use the software, start Excel and load the MassFluxToolkit.xls model file from the File / Open menu. If you are using Excel 2000, you may see a message box that asks you whether you want to disable or enable the macros. For the Toolkit to operate effectively, you must *enable* the macros.

NOTE: Although the 'Transect Calculator' module in the Toolkit uses Microsoft Excel, the 'Learn About Flux' module calls Microsoft Word and Adobe Acrobat pdf documents. Some features in the "Learn about Flux" module may not work unless you have these programs installed on your computer.

Spreadsheet-Related Problems

Backspace doesn't clear cell. Use the delete key on the keyboard or the mouse to clear data.

The buttons won't work. The Mass Flux Toolkit is built in the Excel spreadsheet environment, and to enter data one must click anywhere outside the cell where data was just entered. If you can see the numbers you just entered in the data entry part of Excel above the spreadsheet, the data have not yet been entered. Click on another cell to enter the data.

is displayed in a number box. The cell format is not compatible with the value, (e.g., the number is too big to fit into the window). To fix this, unprotect the sheet. Then, select the cell, pull down the format menu, select *Cells* and click on the *Number* tab. Change the format of the cell until the value is visible. If the values still cannot be read, select the format menu, select *Cells* and click on the *Font* tab. Reduce the font size until the value can be read.

#DIV/0! is displayed in a number box. The most common cause of this problem is that some input data are missing. In some cases, entering a zero in a box will cause this problem. Double check to make certain that data required for your run have been entered in all of the input cells.

#VALUE! is displayed in a number box. The most common cause of this problem is that some input data are missing. Double check to make certain that data required for your run have been entered in all of the input cells and all options have been selected.

Common Error Messages

Unable to Load Help File: The most common error message encountered with Toolkit is the message 'Unable to Open Help File' after clicking on a *Help* button. Depending on the version of Windows you are using, you may get an Excel Dialog Box, a Windows Dialog Box, or you may see Windows Help load and display the error. This problem is related to the ease with which the

Windows Help Engine can find the data file, MassFluxToolkit.HLP. Here are some suggestions (in decreasing order of preference) for helping WinHelp find it:

- If you are asked to find the requested file, do so. The file is called MassFluxToolkit.HLP, and it was installed in the same directory/folder as the Mass Flux Toolkit model file (MassFluxToolkit.xls).
- Use the File/Open menus from within Excel instead of double-clicking on the filename or Program Manager icon to open the Mass Flux Toolkit model file. This sets the *current directory* to the directory containing the Excel file you just opened.

ACKNOWLEDGEMENTS

SourceDK was developed for the Air Force Center for Environmental Excellence, Brooks AFB, San Antonio, Texas by Groundwater Services, Inc.

ESTCP Project Officer:	Dr. Andrea Leeson
AFCEE Project Officer:	Ms. Erica Becvar
Mass Flux Toolkit Developers:	Dr. Shahla Farhat Dr. Charles Newell Groundwater Services, Inc. 2211 Norfolk, Suite. 1000 Houston, Texas 77098 phone: (713) 522-6300 fax: (713) 522-8010 skfarhat@gsi-net.com Mr. Eric Nichols LFR Levine-Fricke Newfields, New Hampshire
Mass Flux Toolkit User's Manual:	Shahla K. Farhat and Charles J. Newell Groundwater Services, Inc.
Cover Art:	Cover image courtesy of LFR Levine-Fricke and the American Petroleum Institute.
Special Thanks to:	American Petroleum Institute
Mass Flux Toolkit Review Team:	M. Vanderford, X. Osorio, T. Nichols, and D. Bailey Groundwater Services, Inc. Houston, Texas
Mass Flux Toolkit Review Team:	P.B. Bedient and A. Zimmer Rice University Houston, Texas
Mass Flux Toolkit Review Team:	J. Atkinson AFCEE Brooks City Base, Houston
Mass Flux Toolkit Review Team:	H. S. Rifai, Ph.D., P.E. University of Houston, Houston, Texas

ACKNOWLEDGEMENTS

**Mass Flux Toolkit Review
Team:**

T. L. Roth
LFR Levine-Fricke
Newfields, New Hampshire



APPENDICES

APPENDIX A.1. PROBABILITY DISTRIBUTIONS

This section describes in greater detail the probability distributions employed in the LHS sampling. The Mass Flux Toolkit offers the user three distribution options: normal, lognormal, and uniform.

A.1.1 Normal Distributions

Normal distributions are defined by the density function

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\left(\frac{(x-\mu)^2}{2\sigma^2}\right)} \quad -\infty < x < \infty$$

where σ is the standard deviation and μ the mean of the distribution. The Toolkit assumes that the values entered in the “Input Data and Grid” screen are the means. The uncertainty analysis requires the user to specify a σ as a percentage of the mean.

A.1.2 Lognormal Distributions

A lognormal distribution is a distribution whose logarithms are normally distributed. The lognormal density function is

$$f(x) = \frac{1}{x\sigma\sqrt{2\pi}} e^{-\left(\frac{(\ln(x)-\mu)^2}{2\sigma^2}\right)} \quad x, \sigma > 0$$

where σ is the standard deviation and μ the mean of the underlying normal distribution.

Lognormal distributions are typically specified in two ways throughout literature (Swiler and Wyss, 2004). One way, as described above, is to use the mean and standard deviation of the underlying normal distribution. The other way is to by using the mean of the lognormal distribution (α) and a term called the “Error Factor”. For a lognormal distribution, the error factor is the ratio of the 95th percentile to the median, or equivalently, the ratio of the median to the 5th percentile. Therefore, the error factor represents the width of a 90% confidence interval around the median.

In terms of the error factor, the relationship between the underlying normal distribution and the lognormal distribution can be described by

$$\sigma = \ln(\text{error factor})/1.645$$

and

$$\mu = \ln(\alpha) - \frac{\sigma^2}{2}$$

where α is the mean of the lognormal distribution, and σ and μ the standard deviation and mean of the underlying normal distribution, respectively.

The Mass Flux Toolkit describes the lognormal distribution using the error factor.

A.1.3 Uniform Distributions

A uniform distribution is specified over a particular interval and implies that all the points within that interval have equal probability of occurring. The uniform probability distribution function is

$$f(x) = \frac{1}{B - A} \quad A \leq x \leq B$$

where A and B are the lower and upper bounds, respectively.

APPENDIX A.2. LATIN HYPERCUBE SAMPLING

A.2.1 Background

In the standard Monte Carlo approach, simple random sampling, a large number of runs (typically 100 to 1000) are required to obtain a meaningful probability distribution for the parameter. For each run of the standard approach, a random number is generated for every value of concentration, hydraulic conductivity, and hydraulic gradient entered by the user. This set of random inputs is then used to create and interpolate the respective grids and mass flux calculated from those grids. Repeating this procedure a large number of times yields a probability distribution of the mass flux from which statistical characteristics such as mean, percentile, and variance can be obtained. However, the standard Monte Carlo technique tends to be time intensive because of the large number of iterations required.

Latin hypercube sampling (LHS) is a type of stratified Monte Carlo sampling. It can be viewed as a method for controlling the upper and lower ends of the distributions used in the analysis such that all portions of the distribution are well represented (U.S. EPA, 1997; Iman and Helton, 1988; Gwo *et al.*, 1996; Helton and Davis, 2002). In LHS, the given range of each variable in $X_1, \dots, X_n$ is divided into j number of equal non-overlapping probability intervals. A random number with respect to the probability density is then obtained for X_i for each j interval. The j values of X_1 that are obtained are then randomly paired with the j values obtained for X_2 and so on until all the j values in X_n are paired (Iman and Helton, 1988). LHS ensures that a minimal number of probability intervals are required to represent the full range of the distribution (Bergin *et al.*, 1999). Additionally, LHS requires fewer simulations than simple random sampling to achieve the same level of precision (U.S. EPA, 1997; Helton and Davis, 2002), hence a fraction of the time involved with simple random sampling.

A.2.2 Mass Flux Toolkit Methodology

For normal and lognormal distributions, the Mass Flux Toolkit applies LHS in evaluating input uncertainty using the following process:

1. The normal probability distribution described by the users input options (or the underlying normal distribution for the lognormal distribution) is divided into 20 intervals of equal probability.
2. A random number is generated from each interval. The numbers are sorted by magnitude and each assigned a rank. Let each set of 20 random numbers represent a LHS set.
3. Step 2 is repeated for each value of concentration, hydraulic conductivity/Darcy velocity, and gradient (if required) provided by the user.
4. Each concentration LHS set is then randomly paired with each Hydraulic Conductivity/Darcy velocity set and a Spearman rank correlation obtained. This process is repeated until a correlation coefficient of < 0.2 is obtained.
5. If hydraulic conductivity is used to calculate the mass flux then, in addition to the above pairing, correlation coefficients of the pairings of concentration and gradient and conductivity and gradient are also obtained. The pairings are continuously randomized until all the correlation coefficients are < 0.2 .
6. For example, let concentration = A, conductivity/Darcy velocity = B, and gradient = C then, the pairings of A, B, and C are randomized until
 - Correlation (A, B) < 0.2
 - Correlation (A, C) < 0.2
 - Correlation (A, B) < 0.2
7. Correlation coefficients are obtained to minimize any undesired pairings.

8. Each of the randomly paired values of concentration, conductivity/Darcy velocity, and gradient is then used to create a grid.
9. Each grid is interpolated (if required) by the interpolation scheme previously chosen by the user and mass flux calculated. This results in 20 mass flux measurements.
10. Steps 1 through 9 are repeated 10 times for the entire LHS application.
11. The minimum, 15th percentile, 50th percentile, 85th percentile, maximum, and variance are then calculated from the 200 mass fluxes calculated.

For uniform distributions:

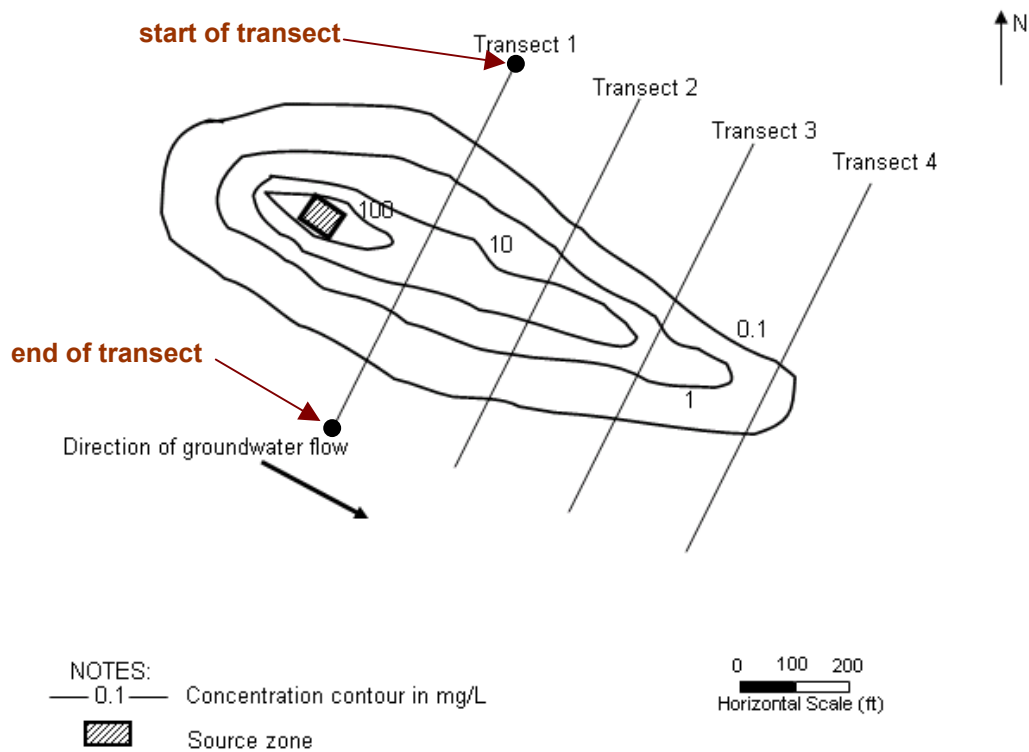
1. Twenty random numbers are generated between the lower and upper bounds specified by the user.
2. The numbers are sorted by magnitude and each assigned a rank.
3. Step 2 is repeated for each value of concentration, hydraulic conductivity/Darcy velocity, and gradient (if required) provided by the user.
4. Steps 4 through 11 for the normal/lognormal distribution are then followed.



EXAMPLES

EXAMPLE 1: MASS FLUX CALCULATION

The following example is obtained from the API's "Groundwater Remediation Strategies Tool" (Newell *et al.*, 2003).



EXAMPLE 1: MASS FLUX CALCULATION

Mass Flux Toolkit Transect Calculator Input

Data Type	Parameter	Value	Source of Data																																																																																				
Transect Data	• Transect 1 From Source:	193 (ft)	• Plume maps																																																																																				
Hydrogeology	• Hydraulic Conductivity: • Hydraulic Gradient:	0.032 (cm/sec) 0.002 (cm/cm)	• Slug-tests results • Static water level measurements																																																																																				
End of Transect	• Transect 1 From Source (start of transect assumed to be left facing downstream):	90 (ft)	• Plume maps																																																																																				
Concentration	• MTBE Concentration <table><thead><tr><th>Name</th><th>Distance of Point from Start of Transect (ft)</th><th>Sampling Interval (ft bgs)</th><th>Plume Top (ft bgs)</th><th>Plume Bottom (ft bgs)</th><th>Conc (mg/L)</th></tr></thead><tbody><tr><td>TRI-2</td><td>10</td><td>5-10</td><td>5</td><td>15</td><td>2.3</td></tr><tr><td>TRI-2</td><td>10</td><td>10-15</td><td>5</td><td>15</td><td>0.47</td></tr><tr><td>TRI-4</td><td>27.5</td><td>5-10</td><td>5</td><td>20</td><td>19.7</td></tr><tr><td>TRI-4</td><td>27.5</td><td>10-15</td><td>5</td><td>20</td><td>7.2</td></tr><tr><td>TRI-4</td><td>27.5</td><td>15-20</td><td>5</td><td>20</td><td>0.34</td></tr><tr><td>TRI-6</td><td>45</td><td>5-10</td><td>5</td><td>20</td><td>87.2</td></tr><tr><td>TRI-6</td><td>45</td><td>10-15</td><td>5</td><td>20</td><td>35.6</td></tr><tr><td>TRI-6</td><td>45</td><td>15-20</td><td>5</td><td>20</td><td>9.5</td></tr><tr><td>TRI-8</td><td>62.5</td><td>5-10</td><td>5</td><td>20</td><td>54.1</td></tr><tr><td>TRI-8</td><td>62.5</td><td>10-15</td><td>5</td><td>20</td><td>15.3</td></tr><tr><td>TRI-8</td><td>62.5</td><td>15-20</td><td>5</td><td>20</td><td>0.67</td></tr><tr><td>TRI-12</td><td>80</td><td>5-10</td><td>5</td><td>15</td><td>4.5</td></tr><tr><td>TRI-12</td><td>80</td><td>10-15</td><td>5</td><td>15</td><td>5.6</td></tr></tbody></table>		Name	Distance of Point from Start of Transect (ft)	Sampling Interval (ft bgs)	Plume Top (ft bgs)	Plume Bottom (ft bgs)	Conc (mg/L)	TRI-2	10	5-10	5	15	2.3	TRI-2	10	10-15	5	15	0.47	TRI-4	27.5	5-10	5	20	19.7	TRI-4	27.5	10-15	5	20	7.2	TRI-4	27.5	15-20	5	20	0.34	TRI-6	45	5-10	5	20	87.2	TRI-6	45	10-15	5	20	35.6	TRI-6	45	15-20	5	20	9.5	TRI-8	62.5	5-10	5	20	54.1	TRI-8	62.5	10-15	5	20	15.3	TRI-8	62.5	15-20	5	20	0.67	TRI-12	80	5-10	5	15	4.5	TRI-12	80	10-15	5	15	5.6	• Plume top based on top of water table • Plume bottom based on top of clay layer below aquifer
Name	Distance of Point from Start of Transect (ft)	Sampling Interval (ft bgs)	Plume Top (ft bgs)	Plume Bottom (ft bgs)	Conc (mg/L)																																																																																		
TRI-2	10	5-10	5	15	2.3																																																																																		
TRI-2	10	10-15	5	15	0.47																																																																																		
TRI-4	27.5	5-10	5	20	19.7																																																																																		
TRI-4	27.5	10-15	5	20	7.2																																																																																		
TRI-4	27.5	15-20	5	20	0.34																																																																																		
TRI-6	45	5-10	5	20	87.2																																																																																		
TRI-6	45	10-15	5	20	35.6																																																																																		
TRI-6	45	15-20	5	20	9.5																																																																																		
TRI-8	62.5	5-10	5	20	54.1																																																																																		
TRI-8	62.5	10-15	5	20	15.3																																																																																		
TRI-8	62.5	15-20	5	20	0.67																																																																																		
TRI-12	80	5-10	5	15	4.5																																																																																		
TRI-12	80	10-15	5	15	5.6																																																																																		

Mass Flux Toolkit Transect Calculator Output

Parameter	Value	Source of Data
Total Mass Flux for Transect 1	105 g/day	See Figure 1-5

Mass Flux Toolkit Modeling Summary:

- The Mass Flux Toolkit was used to estimate the total mass flux and uncertainties associated with that estimate for MTBE at a petroleum refinery.
- The Mass Flux Transect Calculator was used as the primary model to predict the total mass flux because of the availability of site hydrogeological and transect concentration data.

EXAMPLE 1: MASS FLUX CALCULATION

- The Distance of Transect from Source was entered in Section 6.1, hydraulic conductivity in Section 6.4, hydraulic gradient in Section 6.5, and individual transect data in the table. Uniform hydraulic conductivity and gradient fields were chosen across the entire transect. Because the data was collected at various intervals, the Sampling Interval option was selected in Section 6.6.
- A grid refinement of 1 x 1 was used in Section 7 as a conservative measure.
- No interpolation was required for the concentration grid and since uniform hydraulic conductivity and gradient were used, no interpolation was required for these grids either.
- Figure 1-5 shows the total MTBE mass flux calculated across Transect 1.
- A simple uncertainty analysis was performed on the data to determine potential areas of high uncertainty. Figure 1-6 shows the results of the uncertainty analysis.

KEY POINT:

The Mass Flux Toolkit indicates that the total mass groundwater flux across transect 1 is 105 g/day. An uncertainty analysis on the input data shows that of all the sampling points collected, TRI-6 sampling interval 15-20 ft has the largest influence on the total mass flux (23 % contribution to total mass flux).

EXAMPLE 1: MASS FLUX CALCULATION

Input Data and Grid

Site Location and I.D.: Texas

Description: MTBE

4. CHOOSE TRANSECT Transect 1

6. ENTER TRANSECT DATA

6.1 Distance of Transect 1 from Source 193 (ft)

6.2 ☐ Darcy Velocity ☒ Hydraulic Conductivity

6.3 Hydraulic Conductivity Units cm/sec

6.4 Uniform Hydraulic Conductivity? Yes

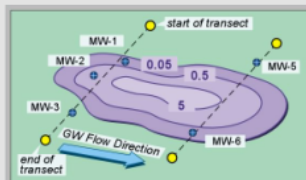
6.5 Uniform Hydraulic Gradient? Yes

5. CHOOSE TIME PERIOD 1

6.6 ☒ Sampling Interval ☐ Mid Point of Sampling Interval

6.4 Hydraulic Conductivity 3.20E-02 (cm/sec)

6.5 Hydraulic Gradient 2.00E-03 (cm/cm)



Data Input Instructions

Enter value directly.

Value calculated by model (Don't enter any data)

Monitoring Point	Distance of Monitoring Point from Start of Transect (ft)	Sampling Interval (ft bgs)		Plume Top (ft bgs)	Plume Bottom (ft bgs)	Concentration (mg/L)	
		Top	Bottom			Constituent A	Constituent B
						MTBE	
1 Start of Transect	0					0	0
2 End of Transect	90					0	0
3 TR1-2	10	5	10	5	15	2.3	
4 TR1-2	10	10	15	5	15	0.47	
5 TR1-4	27.5	5	10	5	20	19.7	
6 TR1-4	27.5	10	15	5	20	7.2	
7 TR1-4	27.5	15	20	5	20	0.34	
8 TR1-6	45	5	10	5	20	87.2	
9 TR1-6	45	10	15	5	20	35.6	
10 TR1-6	45	15	20	5	20	9.5	
11 TR1-8	62.5	5	10	5	20	54.1	
12 TR1-8	62.5	10	15	5	20	15.3	
13 TR1-8	62.5	15	20	5	20	0.67	
14 TR1-12	80	5	10	5	15	4.5	
15 TR1-12	80	10	15	5	15	5.6	

7. CHOOSE GRID (OPTIONAL)

Current Grid: Number of rows 10, Number of columns 7

Refine Grid By: 1, Refined Grid: 10

1, 7

8. SELECT CONSTITUENT FOR CALCULATIONS

☒ MTBE ☐ Constituent B

Next Step:

Continue Data Input

[Back to Transect Calculator Screen](#)

[Clear Screen](#)

[Import MW Data](#)

[Paste Example](#)

[Export MW Data](#)

[Restore Table Formatting](#)

[See CondFlux Grids](#)

[Print](#)

[HELP](#)

Figure 1-1. Input Data and Grid Screen.

EXAMPLE 1: MASS FLUX CALCULATION

Grid Completion: Concentration

Transect 1 Time Period 1. No Interpolation Required (No Space Available in Grid for Interpolation).

Step 10: Interpolate Conc Horizontally		Export Conc Grid	Import Conc Grid	Next Step: View Hydraulic Conductivity Grid
Back to Data Input	Back to Conc Grid	Back to K Grid	Print	

Data Input Instructions

10.80

Enter value directly.
(Values in
italics represent
interpolated values.)



Top/Bottom of plume.
(Don't enter any
data).

MTBE Concentrations (mg/L)

Distance from Edge of Transect (ft)

	Start of Transect <i>0.0</i>	TR1-2 <i>10.0</i>	TR1-4 <i>27.5</i>	TR1-6 <i>45.0</i>	TR1-8 <i>62.5</i>	TR1-12 <i>80.0</i>	End of Transect <i>90.0</i>
5.0	0	2.30E+00	1.97E+01	8.72E+01	5.41E+01	4.50E+00	0
6.5	0	2.30E+00	1.97E+01	8.72E+01	5.41E+01	4.50E+00	0
8.0	0	2.30E+00	1.97E+01	8.72E+01	5.41E+01	4.50E+00	0
9.5	0	4.70E-01	7.20E+00	3.56E+01	1.53E+01	5.60E+00	0
11.0	0	4.70E-01	7.20E+00	3.56E+01	1.53E+01	5.60E+00	0
12.5	0	4.70E-01	7.20E+00	3.56E+01	1.53E+01	5.60E+00	0
14.0	0	4.70E-01	7.20E+00	3.56E+01	1.53E+01	5.60E+00	0
15.5			3.40E-01	9.50E+00	6.70E-01		
17.0			3.40E-01	9.50E+00	6.70E-01		
18.5			3.40E-01	9.50E+00	6.70E-01		
20.0							

Figure 1-2. Concentration Grid

Grid Completion: Hydraulic Conductivity

Transect 1 Time Period 1. Constant Conductivity: No Interpolation Required

Step 10: Interpolate K Horizontally

Export K Grid

Import K Grid

Next Step:
View Hydraulic
Gradient Grid

Back to Data Input

Back to Conc Grid

Back to K Grid

Print

HELP

Data Input Instructions

10.80 → Enter value directly.
(Values in italics represent interpolated values.)

→ Top/Bottom of plume.
(Don't enter any data).

Hydraulic Conductivity (cm/sec)

Distance from Edge of Transect (ft)

	Start of Transect <i>0.0</i>	TR1-2 <i>10.0</i>	TR1-4 <i>27.5</i>	TR1-6 <i>45.0</i>	TR1-8 <i>62.5</i>	TR1-12 <i>80.0</i>	End of Transect <i>90.0</i>
<i>5.0</i>	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02
<i>6.5</i>	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02
<i>8.0</i>	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02
<i>9.5</i>	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02
<i>11.0</i>	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02
<i>12.5</i>	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02
<i>14.0</i>	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02	3.20E-02
<i>15.5</i>			3.20E-02	3.20E-02	3.20E-02		
<i>17.0</i>			3.20E-02	3.20E-02	3.20E-02		
<i>18.5</i>			3.20E-02	3.20E-02	3.20E-02		
<i>20.0</i>							

Figure 1-3. Hydraulic Conductivity Grid

EXAMPLE 1: MASS FLUX CALCULATION

Grid Completion: Hydraulic Gradient

Transect 1 Time Period 1. Constant Gradient: No Interpolation Required

Step 10: Interpolate i Horizontally
Export i Grid
Import i Grid

Next Step:
Calculate Mass Flux

Back to Data Input
Back to Conc Grid
Back to K Grid
Print
HELP

Data Input Instructions

10.80 → Enter value directly.
(Values in italics represent interpolated values.)

 → Top/Bottom of plume.
(Don't enter any data).

Hydraulic Gradient (cm/cm)

Distance from Edge of Transect (ft)

	Start of Transect <i>0.0</i>	TR1-2 <i>10.0</i>	TR1-4 <i>27.5</i>	TR1-6 <i>45.0</i>	TR1-8 <i>62.5</i>	TR1-12 <i>80.0</i>	End of Transect <i>90.0</i>
<i>5.0</i>	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03
<i>6.5</i>	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03
<i>8.0</i>	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03
<i>9.5</i>	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03
<i>11.0</i>	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03
<i>12.5</i>	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03
<i>14.0</i>	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03	2.00E-03
<i>15.5</i>			2.00E-03	2.00E-03	2.00E-03		
<i>17.0</i>			2.00E-03	2.00E-03	2.00E-03		
<i>18.5</i>			2.00E-03	2.00E-03	2.00E-03		
<i>20.0</i>							

Figure 1-4. Hydraulic Gradient Grid

EXAMPLE 1: MASS FLUX CALCULATION

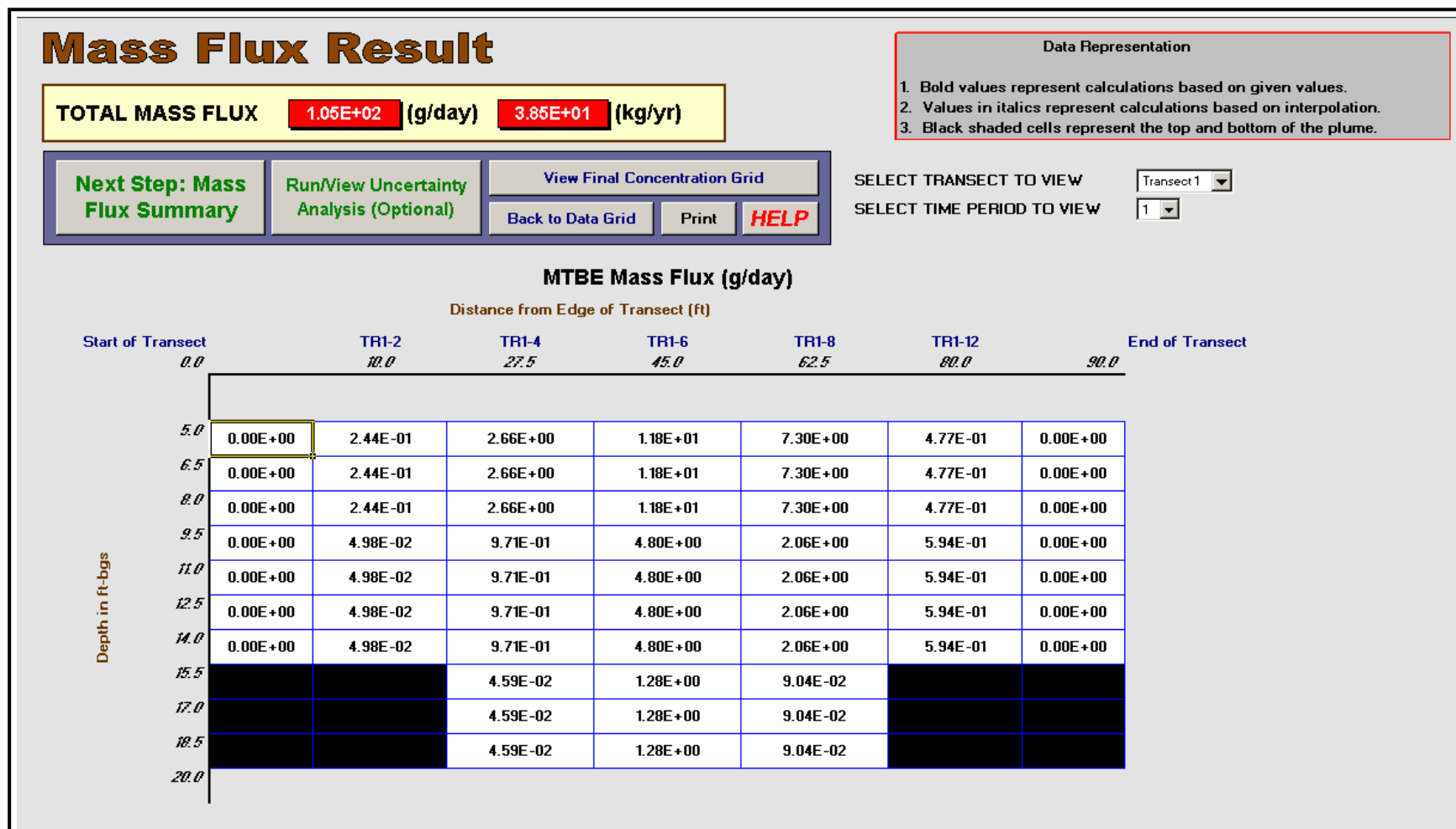


Figure 1-5. Mass Flux Results Grid

EXAMPLE 1: MASS FLUX CALCULATION

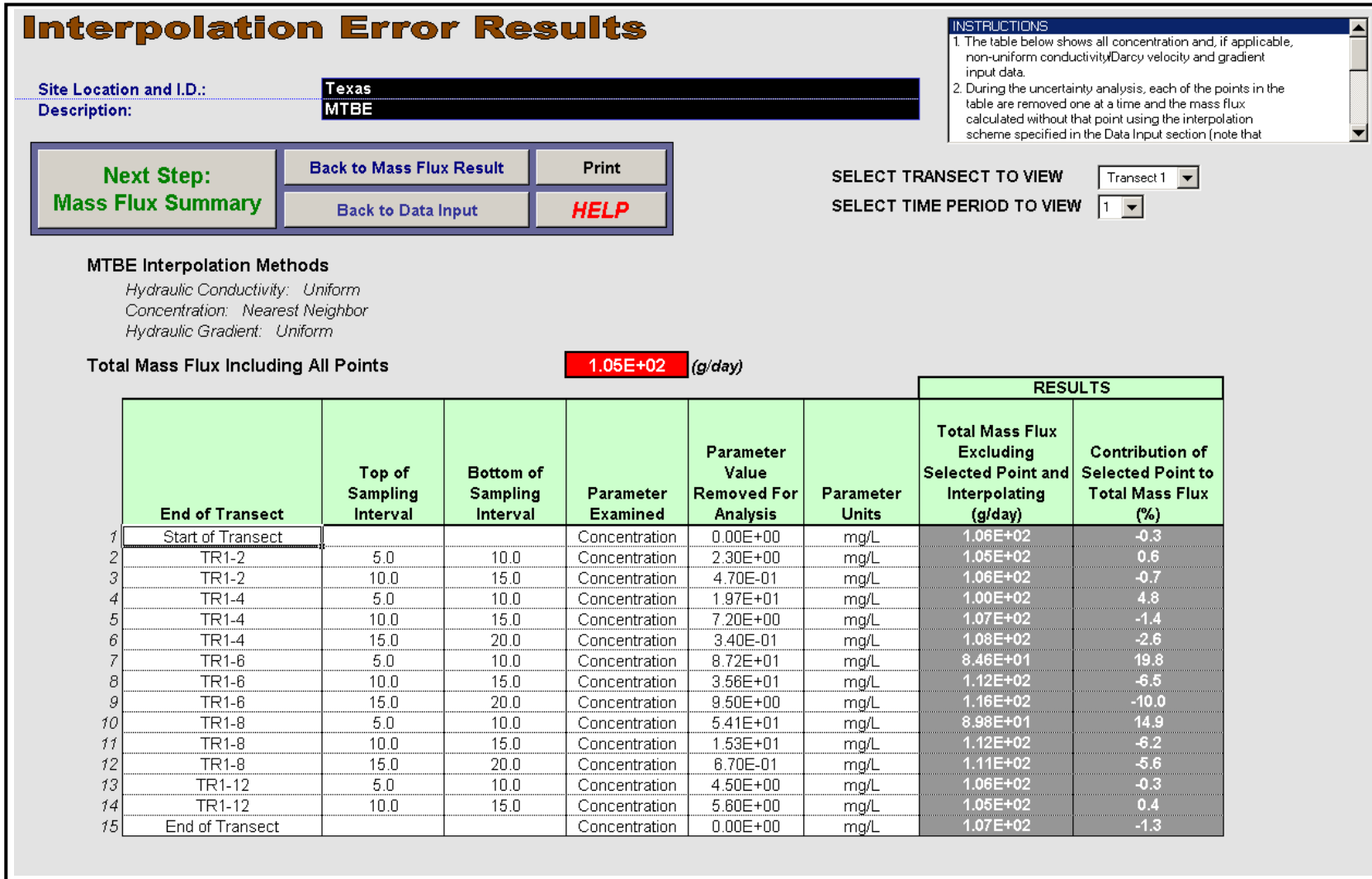
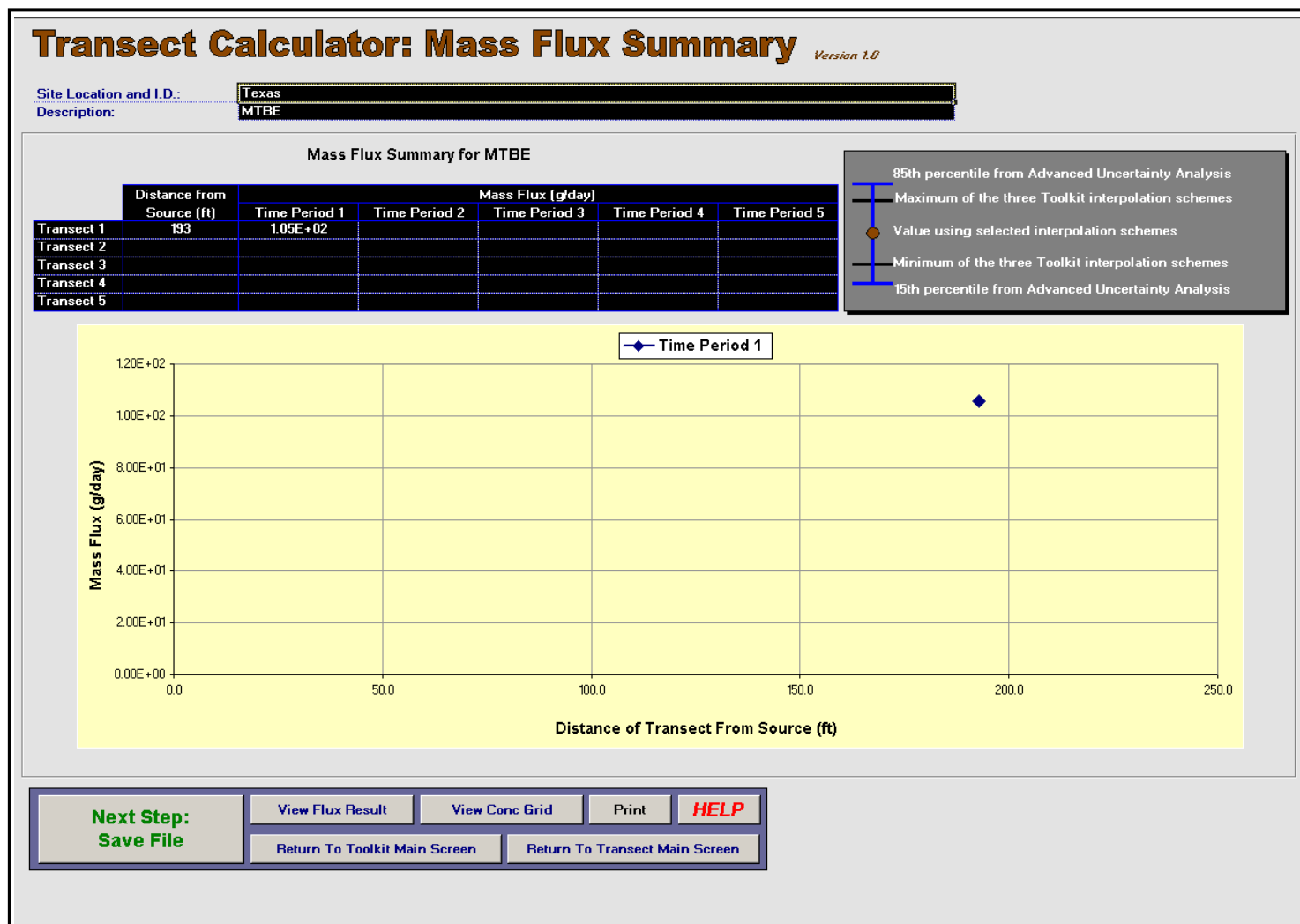


Figure 1-6. Simple Uncertainty Analysis

EXAMPLE 1: MASS FLUX CALCULATION



EXAMPLE 2: MTBE CONCENTRATION AT CONTROL POINT

The following example is obtained from the API's "Groundwater Remediation Strategies Tool" (Newell *et al.*, 2003).

Total Mass Flux is Calculated Using Data Provided in Example 1. Transect 1 was used as a conservative pick for the calculation of the control point concentration and does not assume any natural attenuation.

Mass Flux Toolkit Receptor Impact – Wells Input

Data Type	Parameter	Value
Supply Well	• Flow rate:	10 (gpm)

Mass Flux Toolkit Receptor Impact – Wells Output

Parameter	Value	Source of Data
• Total Mass Flux for Transect 1	• 105 g/day	See Figure 1-5 of Example 1
• Concentration at Control Point	• 1.94 mg/L	See Figure 2-1

Mass Flux Toolkit Modeling Summary:

- The Mass Flux Toolkit was used to estimate the total mass flux and uncertainties associated with that estimate for MTBE at a petroleum refinery (See Example 1).
- The Mass Flux Transect Calculator was used as the primary model to predict the total mass flux because of the availability of site hydrogeological and transect concentration data (See Example 1).
- The Distance of Transect from Source was entered in Section 6.1, hydraulic conductivity in Section 6.4, hydraulic gradient in Section 6.5, and individual transect data in the table. Uniform hydraulic conductivity and gradient fields were chosen across the entire transect. Because the data was collected at various intervals, the Sampling Interval option was selected in Section 6.6 (See Example 1).
- A grid refinement of 1 x 1 was used in Section 7 (See Example 1).
- No interpolation was required for the concentration grid and since uniform hydraulic conductivity and gradient were used, no interpolation was required for these grids either (See Example 1).
- Figure 1-5 shows the total MTBE mass flux calculated across Transect 1 (See Example 1).
- The Impact to Receptor-Wells model was used to calculate the concentration of MTBE at the control point.
- Transect 1 and Time Period 1 were selected in Section 1 of the Impact to Receptor-Wells input screen. The flow rate of the supply well was also entered in Section 1.

KEY POINT:

The Mass Flux Toolkit indicates that the total groundwater mass flux across transect 1 is 105 g/day which results in a concentration of 1.94 mg/L at the control point. This value assumes the plume is at a steady-state condition. Some corrective action measures may be required to reduce the control point concentration.

Receptor Impact Worksheet - Wells Version 1.0 Beta

Site Location and I.D.: Texas

Description: MTBE

1. CONSTITUENT CONCENTRATION

☒ MTBE ☐ Constituent B

Transect of Interest: Transect 1

Time Period of Interest: 1

Discharge Rate for Each Supply Well: 1.00E+01 gpm

Total Mass Flux (Calculated From Mass Flux Transect Method): 1.05E+02 (g/day)

Maximum Constituent Concentration in Water Extracted from Supply Well: 1.94E+00 (mg/L)

2. CAPTURE ZONE (OPTIONAL)

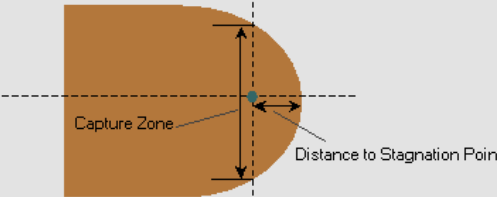
Number of Supply Wells:

Aquifer Thickness: (ft)

Darcy Velocity for Transect: 6.40E-05 (cm/sec)

Capture Zone of Supply Well(s): No Data (ft)

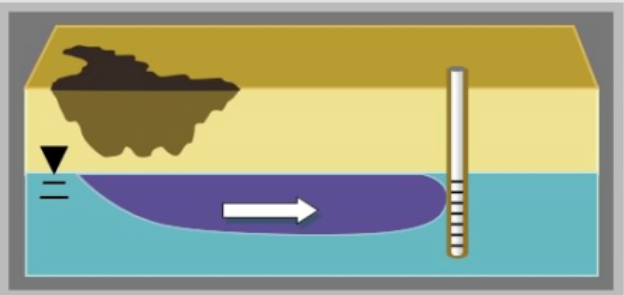
Distance of Supply Well from Stagnation Point: No Data (ft)



Data Input Instructions:

10.80 → Enter value directly.

10.80 → Value calculated by model. (Don't enter any data.)



Return To Main Screen
Clear Screen
Paste Example
Save File
Load File
Print
HELP

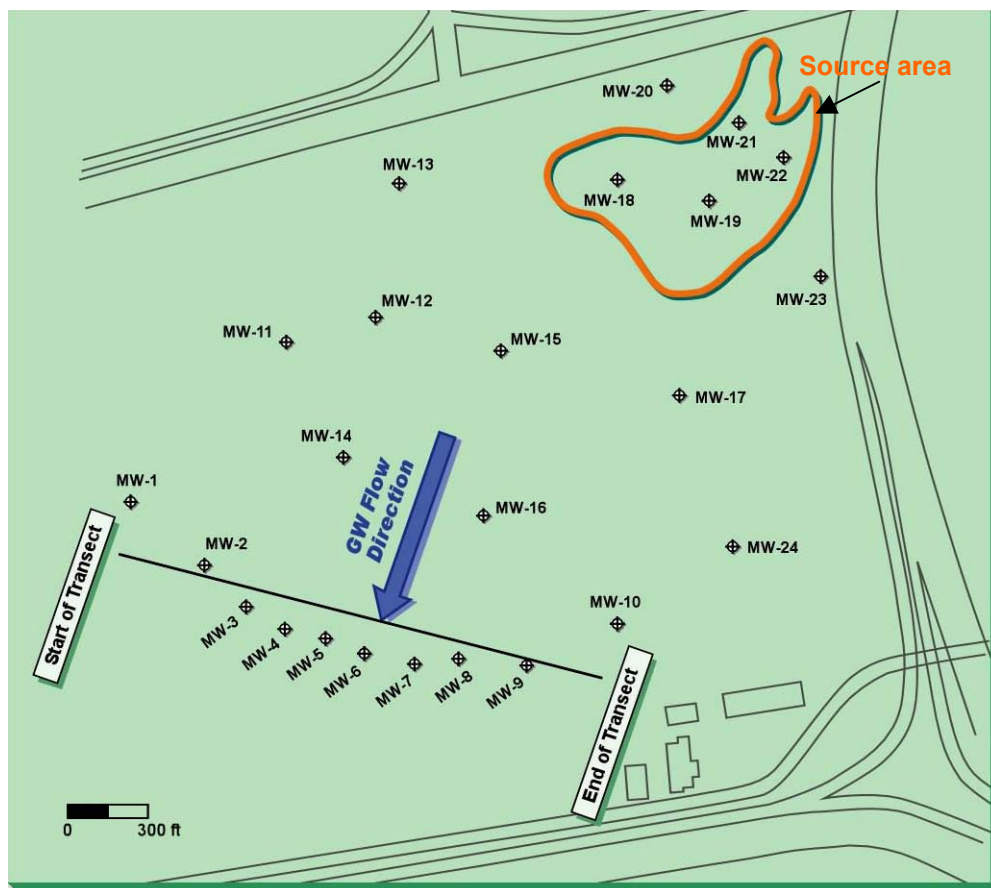
Figure 2-1. Control Point Concentration.

CASE STUDY

CASE STUDY: MTBE AND TBA

Data for the following case study was provided by LFR Levine-Fricke (personal communication with T. L. Roth and E.M. Nichols at LFR Levine-Fricke, February 2006). They compared methyl tert-butyl ether (MTBE) and tertiary butyl alcohol (TBA) mass flux calculated using the Toolkit to a manual calculation based on a site-specific grid using an interpolation of concentration and a detailed sequential indicator kriging interpolation of hydraulic conductivity.

This case study documents the comparison of mass flux calculations. Note that the following site figure is for demonstration only and does not represent the actual site.



Mass Flux Transect Calculator Input

Data Type	Parameter					Value				Source of Data
Transect Data	• Transect 1 From Source:					1700 (ft)				• Plume map
Hydrogeology	• Hydraulic Conductivity: • Hydraulic Gradient:					See table below See table below				• Slug-tests results/estimations • Static water level measurements
End of Transect	• Transect 1 From Source (start of transect assumed to be at the right facing downstream):					1700 (ft)				• Plume map
Data	Distance of Point from Start of Transect (ft) Name Sampling Interval (ft bgs) Plume Top (ft bgs) Plume Bottom (ft bgs) K (ft/d) i (ft/ft) MTBE Conc (mg/L) TBA Conc (mg/L)									• Plume top based on top of water table • Plume bottom based on top of clay layer below aquifer
	MW-1	100	5-20	7.14	81.30	150	0.00071	0.5	10	
	MW-1	100	33-38	7.14	81.30	22	0.00071	0.5	10	
	MW-1	100	51-56	7.14	81.30	27	0.00071	0.5	10	
	MW-1	100	66-71	7.14	81.30	1	0.00071	0.5	10	
	MW-2	325	7-22	11.23	92.00	150	0.0021	2.8	55	
	MW-2	325	40-45	11.23	92.00	26	0.0021	86	310	
	MW-2	325	62-67	11.23	92.00	114	0.0021	7.2	890	
	MW-2	325	77-82	11.23	92.00	1	0.0021	0.5	10	
	MW-3	500	10-25	15.81	92.00	31	0.0021	21	10	
	MW-3	500	38-43	15.81	92.00	66	0.0021	14	10	
	MW-3	500	58-63	15.81	92.00	150	0.0021	17	10	
	MW-3	500	77-82	15.81	92.00	1	0.0021	4.6	30	
	MW-4	665	15-30	21.15	95.00	21	0.0021	11	0.01	
	MW-4	665	44-49	21.15	95.00	50	0.0021	3.7	0.01	
	MW-4	665	63-68	21.15	95.00	87	0.0021	3	0.01	
	MW-4	665	80-85	21.15	95.00	1	0.0021	0.5	0.01	

CASE STUDY: MTBE AND TBA

Name	Distance of Point from Start of Transect (ft)	Sampling Interval (ft bgs)	Plume Top (ft bgs)	Plume Bottom (ft bgs)	K (ft/d)	i (ft/ft)	MTBE Conc (mg/L)	TBA Conc (mg/L)
MW-5	805	20-35	24.91	96	33	0.0021	12	0.01
MW-5	805	47-52	24.91	96	57	0.0021	11	0.01
MW-5	805	65-70	24.91	96	150	0.0021	4.2	0.01
MW-5	805	81-86	24.91	96	1	0.0021	0.5	0.01
MW-6	1005	24-39	29.55	77	150	0.0019	6.2	0.01
MW-6	1005	47-52	29.55	77	58	0.0019	5.2	0.01
MW-6	1005	62-67	29.55	77	1	0.0019	0.5	0.01
MW-7	1185	30-45	35.63	82	44	0.0019	6.9	0.01
MW-7	1185	52-57	35.63	82	51	0.0019	7.4	0.01
MW-7	1185	67-72	35.63	82	1	0.0019	0.5	0.01
MW-8	1430	29-44	32.54	81	44	0.0019	4.2	0.01
MW-8	1430	51-56	32.54	81	51	0.0019	6.3	0.01
MW-8	1430	66-71	32.54	81	1	0.0019	0.5	0.01

Mass Flux Transect Calculator Output

Data Type	Parameter	Value	
LFR Levine-Fricke Independent Estimate	Total Mass Flux for Transect 1	MTBE 1.7 g/day	TBA 9.4 g/day
Toolkit Estimates	Total Mass Flux for Transect 1	MTBE	TBA
	MTBE: Figures 3-8 and 3-9; 3-19 and 3-20; and 3-30 and 3-31	Natural Neighbor Interpolation 2.5 g/day	21.2 g/day
	TBA: Figures 3-37 and 3-38; 3-44 and 3-45; and 3-51 and 3-52	Linear Interpolation 2.9 g/day	20.4 g/day
		Log Transformation 1.7 g/day	9.3 g/day

Mass Flux Toolkit Modeling Summary:

- The Mass Flux Toolkit was used to estimate the total mass flux and uncertainties associated with that estimate for MTBE and TBA at a petroleum refinery.
- The Mass Flux Transect Calculator was used as the primary model to predict the total mass flux because of the availability of site hydrogeological and transect concentration data.
- The Distance of Transect from Source was entered in Section 6.1, hydraulic conductivity in Section 6.4, hydraulic gradient in Section 6.5, and individual transect data in the table. Because the data was collected at various intervals, the Sampling Interval option was selected in Section 6.6.
- A grid refinement of 2 x 2 (to match the LFR Levine-Fricke grid) was used in Section 7.
- Mass flux was calculated using each of the three interpolation techniques available in the Toolkit for comparison purposes.
- Figure 3-1 shows the input data for the Toolkit.
- Figures 3-2 and 3-3, 3-13 and 3-14, and 3-24 and 3-25 show the final MTBE concentration grids calculated using the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.
- Figures 3-4 and 3-5, 3-15 and 3-16, and 3-26 and 3-27 show the final hydraulic conductivity grids calculated using the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.
- Figures 3-6 and 3-7, 3-17 and 3-18, and 3-28 and 3-29 show the final hydraulic gradient grids calculated using the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.
- Figures 3-8 and 3-9, 3-19 and 3-20, and 3-30 and 3-31 show the total MTBE mass flux calculated using the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.
- A simple uncertainty analysis was performed on the data to determine potential areas of high uncertainty. Figures 3-10 and 3-11, 3-21 and 3-22, and 3-32 and 3-33 show the results of the uncertainty analysis for MTBE for the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.
- Figures 3-12, 3-23, and 3-34 show the MTBE Mass Flux Summary results for the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.
- Figures 3-35 and 3-36, 3-42 and 3-43, and 3-49 and 3-50 show the final TBA concentration grids calculated using the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.
- Figures 3-37 and 3-38, 3-44 and 3-45, and 3-51 and 3-52 show the total TBA mass flux calculated using the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.

- Figures 3-39 and 3-40, 3-46 and 3-47, and 3-53 and 3-54 show the results of the uncertainty analysis for TBA for the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.
- Figures 3-41, 3-48, and 3-55 show the TBA Mass Flux Summary results for the nearest neighbor interpolation, linear interpolation, and log transformation, respectively.

KEY POINTS:

The total mass groundwater flux across transect 1 obtained using the log transformation for all concentration, conductivity, and gradient grids of 1.7 g/day for MTBE and 9.3 g/day for TBA was in agreement with the LFR Levine-Fricke manual calculation of 1.7 g/day for MTBE and 9.4 g/day for TBA.

For MTBE log transformation, an uncertainty analysis on the input data shows that of all the sampling points collected, concentration at MW-2 sampling interval 7-22 ft has the largest influence on the total mass flux (87 % contribution to total mass flux). Hydraulic conductivity at MW-2 sampling interval 40-45 ft has the second largest influence on the total mass flux (68 % contribution to total mass flux).

For the MTBE nearest neighbor interpolation, hydraulic conductivity at MW-2 sampling interval 40-45 ft has the largest influence on the total mass flux (62 % contribution to total mass flux) while concentration at MW-2 sampling interval 7-22 ft has the second largest influence on the total mass flux (53 % contribution to total mass flux).

For MTBE linear interpolation, concentration at MW-2 sampling interval 7-22 ft has the largest influence on the total mass flux (65 % contribution to total mass flux) while hydraulic conductivity at MW-2 sampling interval 40-45 ft has the second largest influence on the total mass flux (55 % contribution to total mass flux).

For TBA log transformation, an uncertainty analysis on the input data (log transformation) shows that of all the sampling points collected, hydraulic conductivity at MW-2 sampling interval 40-45 ft has the largest influence on the total mass flux (68 % contribution to total mass flux). Concentration at MW-2 sampling interval 62-67 ft also has a large influence on the total mass flux (56 % contribution to total mass flux).

For TBA nearest neighbor interpolation, concentration at MW-2 sampling interval 62-67 ft has the largest influence on the total mass flux (69 % contribution to total mass flux) while hydraulic conductivity at the same location has the second largest influence on the total mass flux (55 % contribution to total mass flux).

For TBA linear interpolation, concentration at MW-2 sampling interval 62-67 ft has the largest influence on the total mass flux (55 % contribution to total mass flux) while hydraulic conductivity at the same location has the second largest influence on the total mass flux (49 % contribution to total mass flux).

In summary, different methods of interpolation can result in different total mass flux calculations. In this case, a difference of a factor of 2 was observed for TBA calculations.

Input Data and Grid

Site Location and I.D.: LFR Site
Description: MTBE and TBA

4. CHOOSE TRANSECT Transect 1 **5. CHOOSE TIME PERIOD** 1

6. ENTER TRANSECT DATA

6.1 Distance of Transect 1 from Source 1700 (ft)

6.2 ☐ Darcy Velocity ☒ Hydraulic Conductivity **6.6** ☒ Sampling Interval ☐ Mid Point of Sampling Interval

6.3 Hydraulic Conductivity Units ft/d

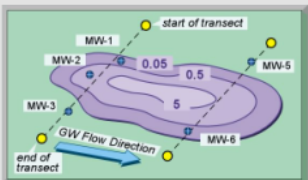
6.4 Uniform Hydraulic Conductivity? No

6.5 Uniform Hydraulic Gradient? No

Monitoring Point	Distance of Monitoring Point from Start of Transect (ft)	Sampling Interval (ft bgs)		Plume Top (ft bgs)	Plume Bottom (ft bgs)	Hydraulic Conductivity (ft/d)	Hydraulic Gradient (ft/ft)	Concentration (ug/L)	
		Top	Bottom					Constituent A	Constituent B
								MTBE	TBA
1 Start of Transect	0							0	0
2 End of Transect	1700							0	0
3 MW-1	100	5	20	7.14	81.3	150	0.00071	0.5	10
4 MW-1	100	33	38	7.14	81.3	22	0.00071	0.5	10
5 MW-1	100	51	56	7.14	81.3	27	0.00071	0.5	10
6 MW-1	100	66	71	7.14	81.3	1	0.00071	0.5	10
7 MW-2	325	7	22	11.23	92	150	0.002133	2.8	55
8 MW-2	325	40	45	11.23	92	26	0.002133	86	310
9 MW-2	325	62	67	11.23	92	114	0.002133	7.2	890
10 MW-2	325	77	82	11.23	92	1	0.002133	0.5	10
11 MW-3	500	10	25	15.81	92	31	0.002133	21	10
12 MW-3	500	38	43	15.81	92	66	0.002133	14	10
13 MW-3	500	58	63	15.81	92	150	0.002133	17	10
14 MW-3	500	77	82	15.81	92	1	0.002133	4.6	30
15 MW-4	665	15	30	21.15	95	21	0.002133	11	0.01

Data Input Instructions

Enter value directly.
 Value calculated by model
 (Don't enter any data)



7. CHOOSE GRID (OPTIONAL)

Current Grid	Refine Grid By	Refined Grid
Number of rows 10	2	20
Number of columns 10	2	19

8. SELECT CONSTITUENT FOR CALCULATIONS

☒ MTBE ☐ TBA

Next Step:
Continue Data Input

Back to Transect Calculator Screen

Import MW Data

Export MW Data

See ConoFlux Grids

Clear Screen

Paste Example

Restore Table Formatting

Print

HELP

Figure 3-1. Input Data and Grid Screen.

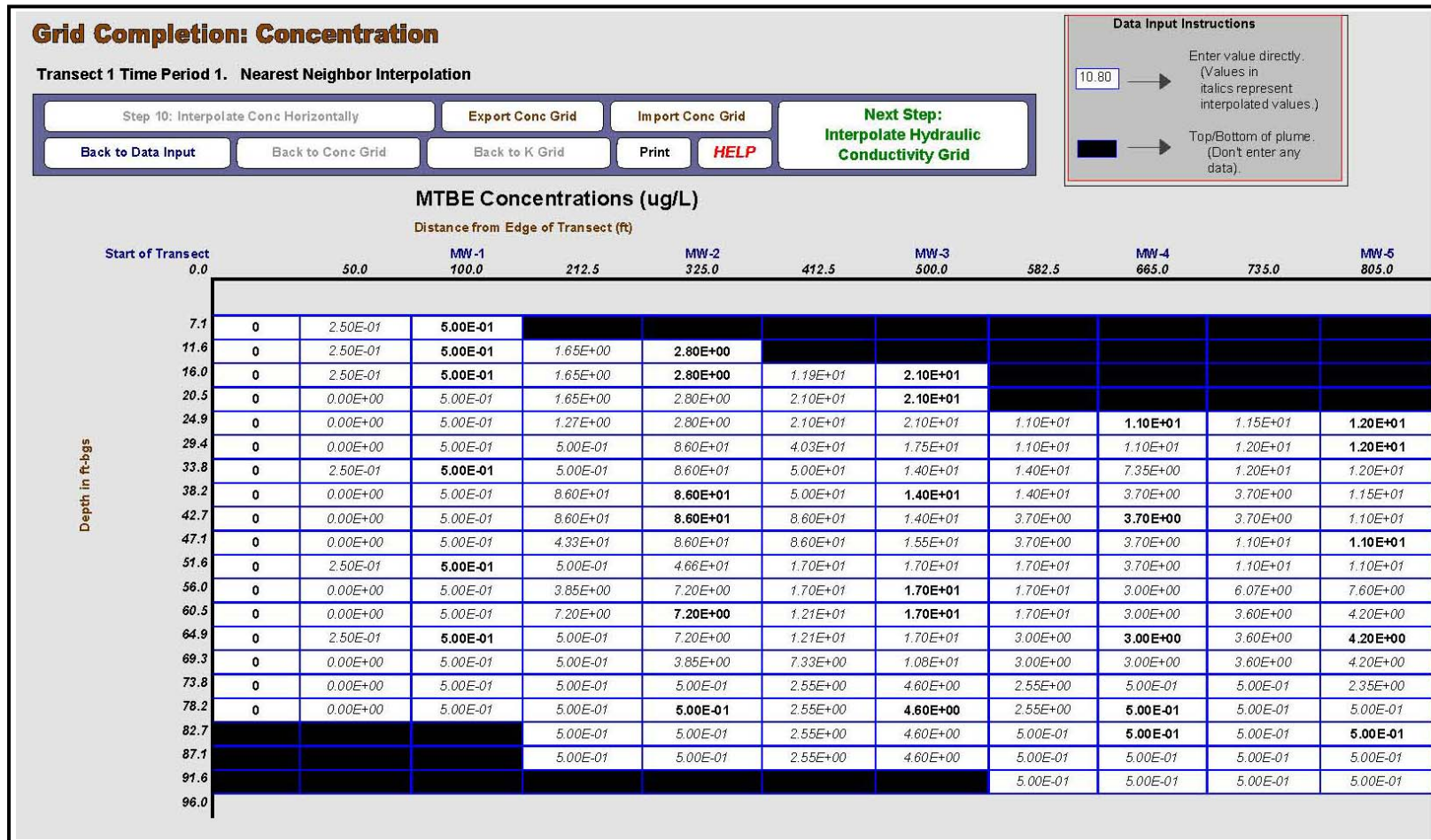


Figure 3-2. MTBE Nearest Neighbor Interpolation: Concentration Grid – Page 1

CASE STUDY: MTBE AND TBA

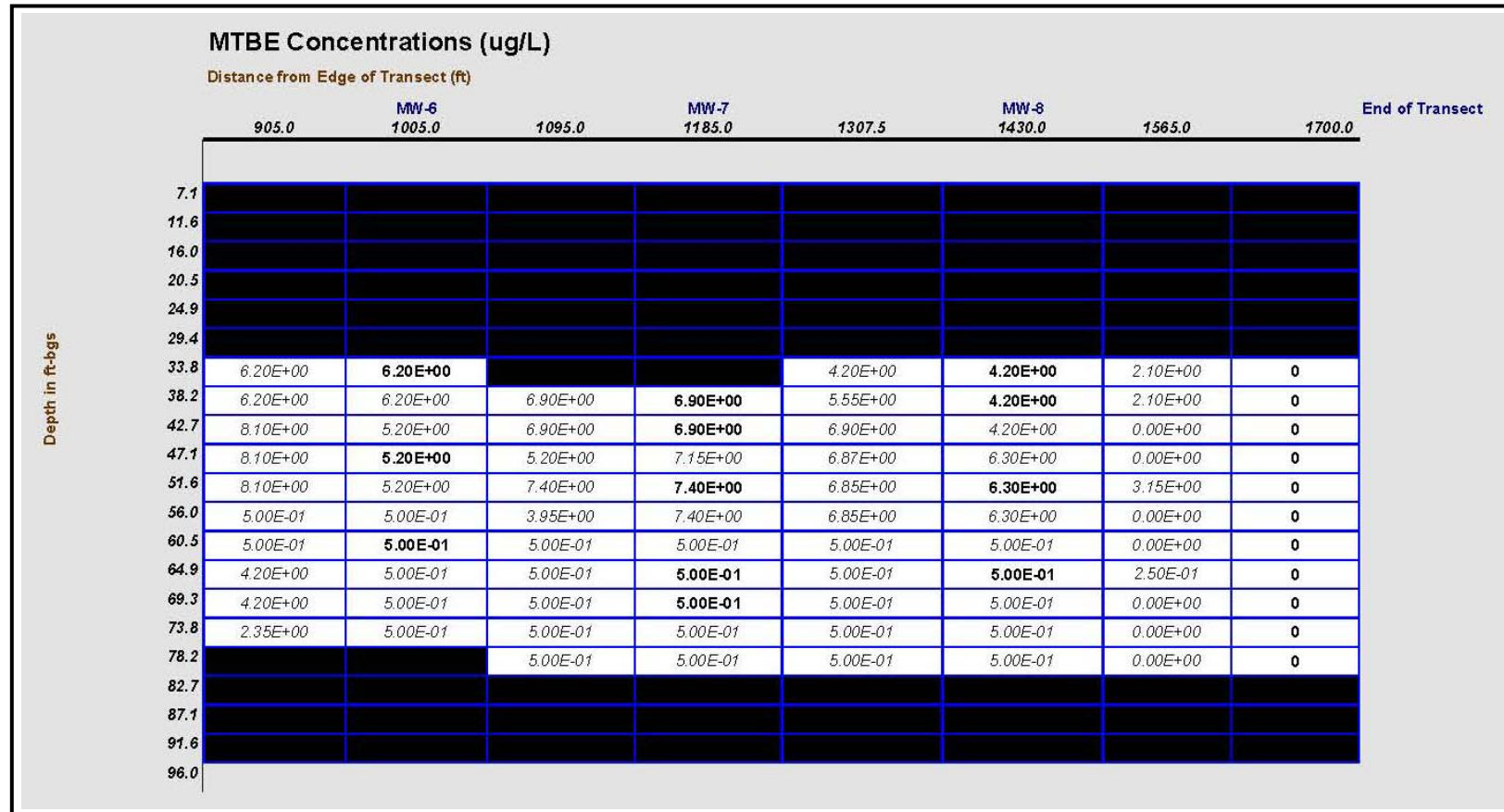


Figure 3-3. MTBE Nearest Neighbor Interpolation: Concentration Grid – Page 2

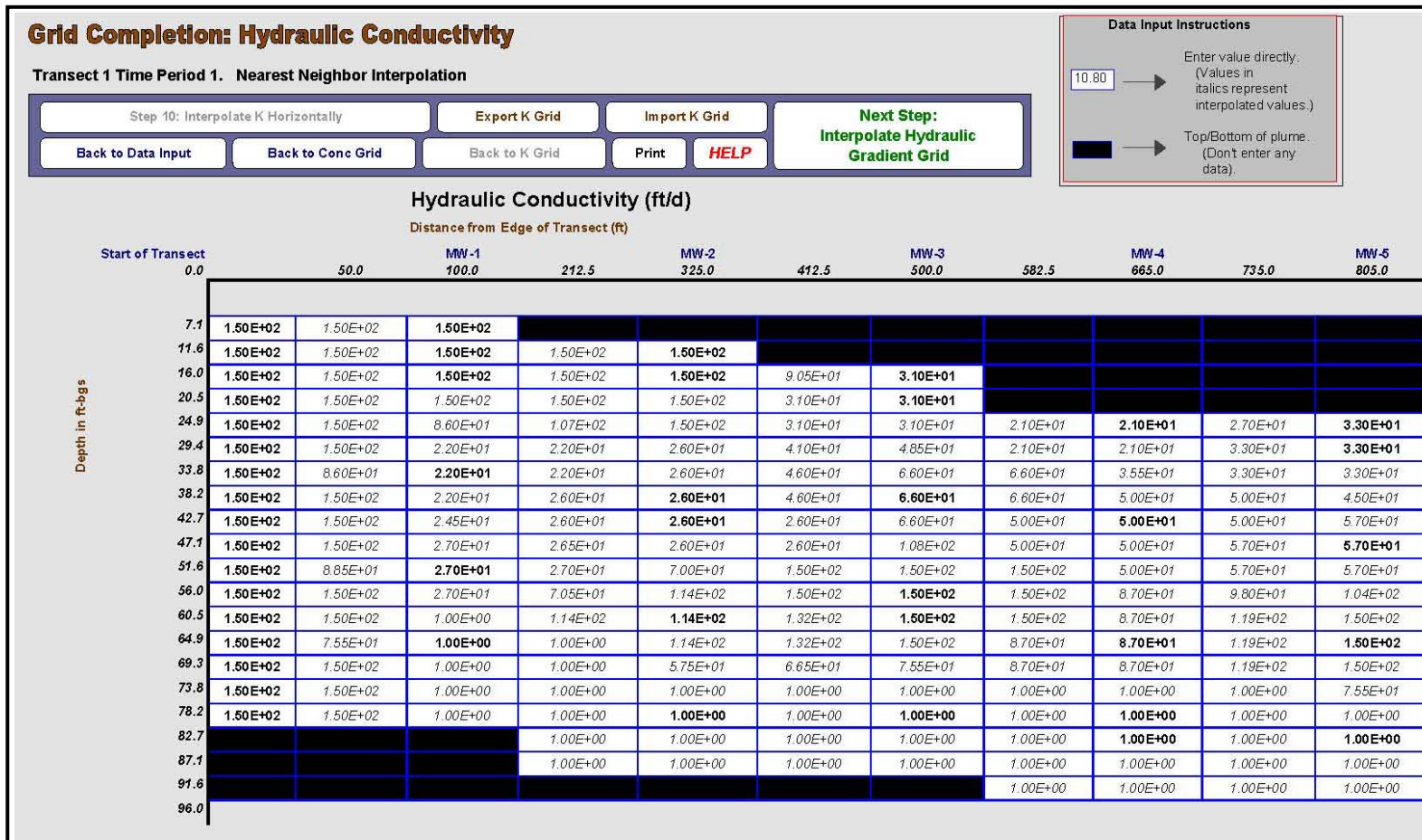


Figure 3-4. Nearest Neighbor Interpolation: Hydraulic Conductivity Grid – Page 1

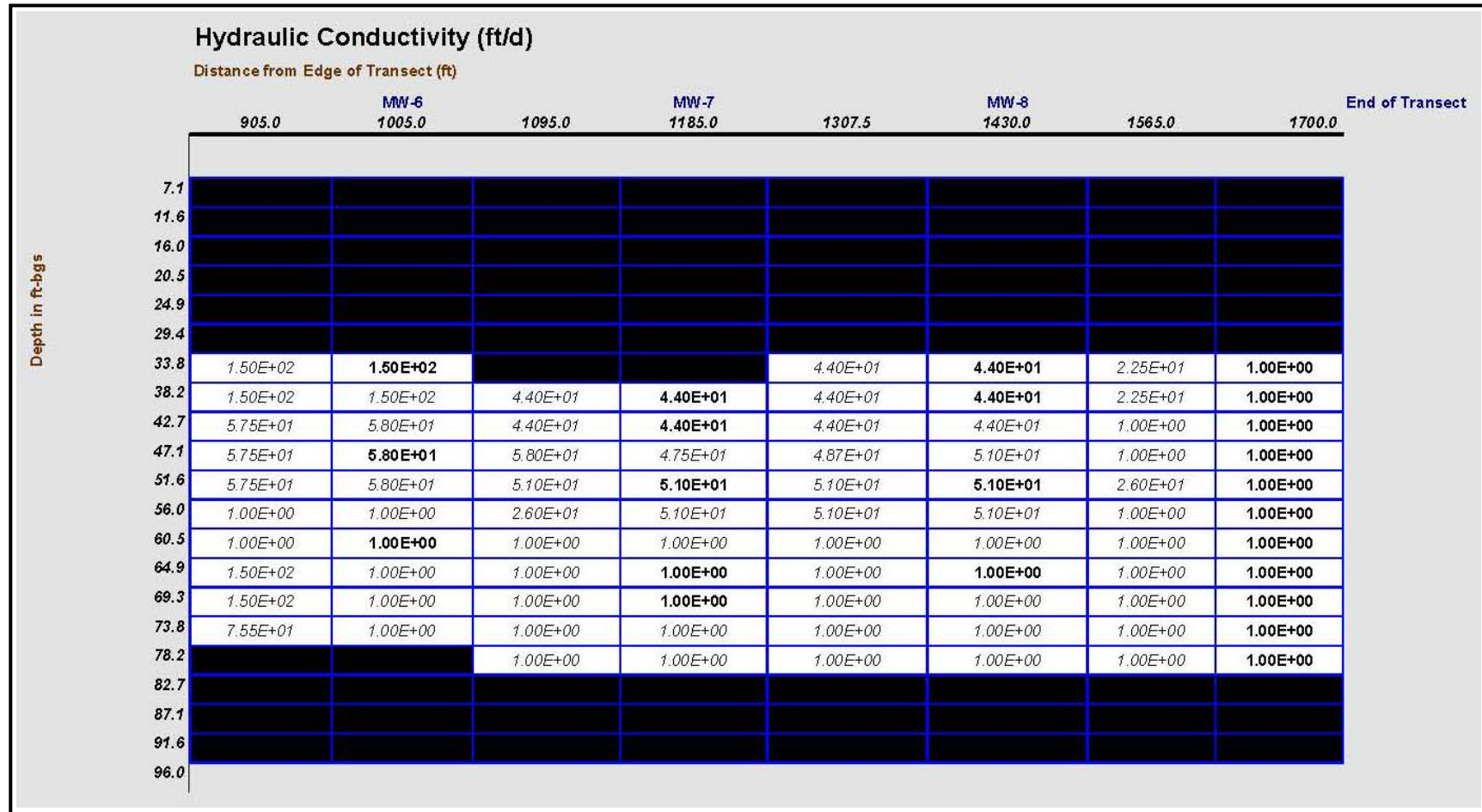


Figure 3-5. Nearest Neighbor Interpolation: Hydraulic Conductivity Grid – Page 2

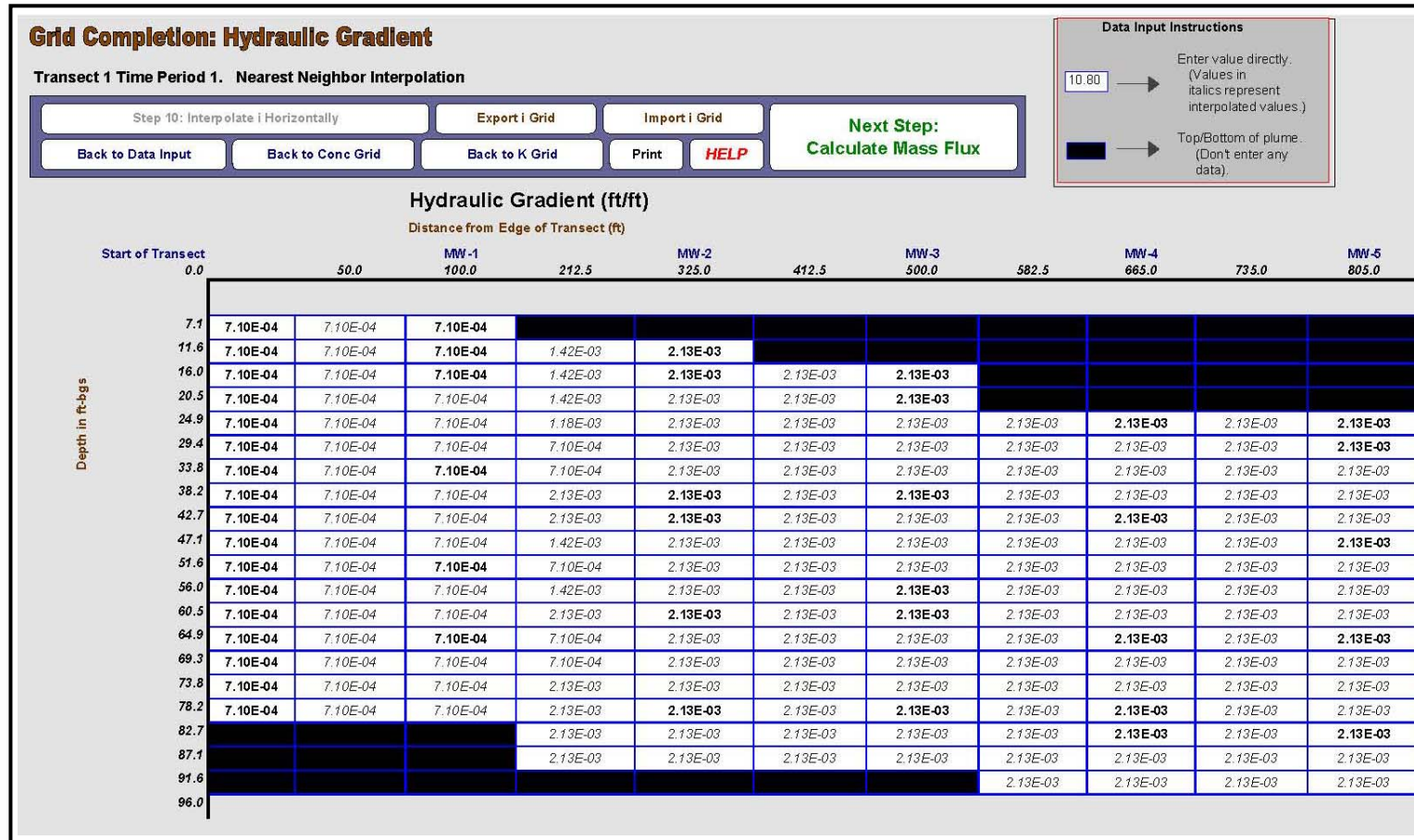


Figure 3-6. Nearest Neighbor Interpolation: Hydraulic Gradient Grid – Page 1

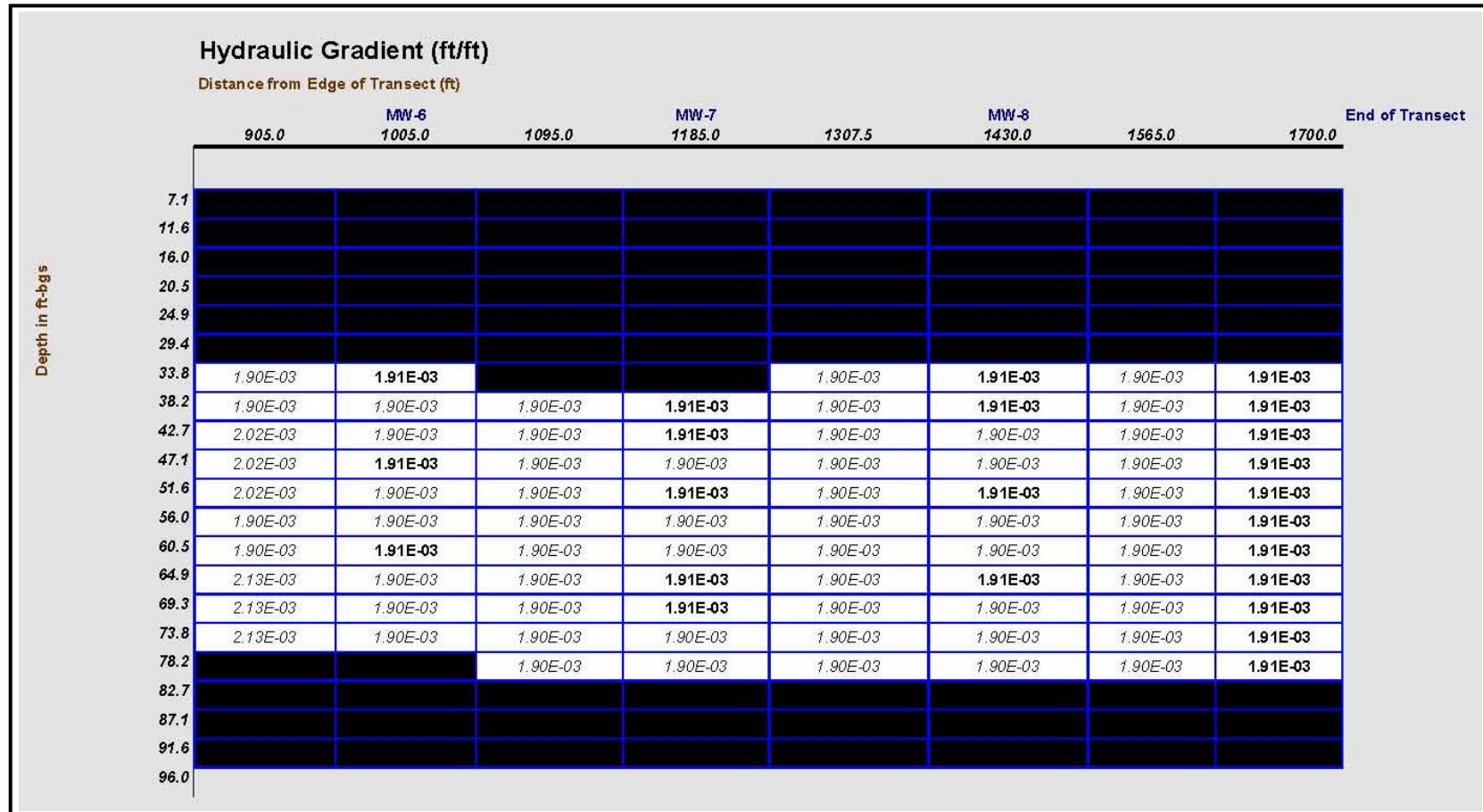


Figure 3-7. Nearest Neighbor Interpolation: Hydraulic Gradient Grid – Page 2

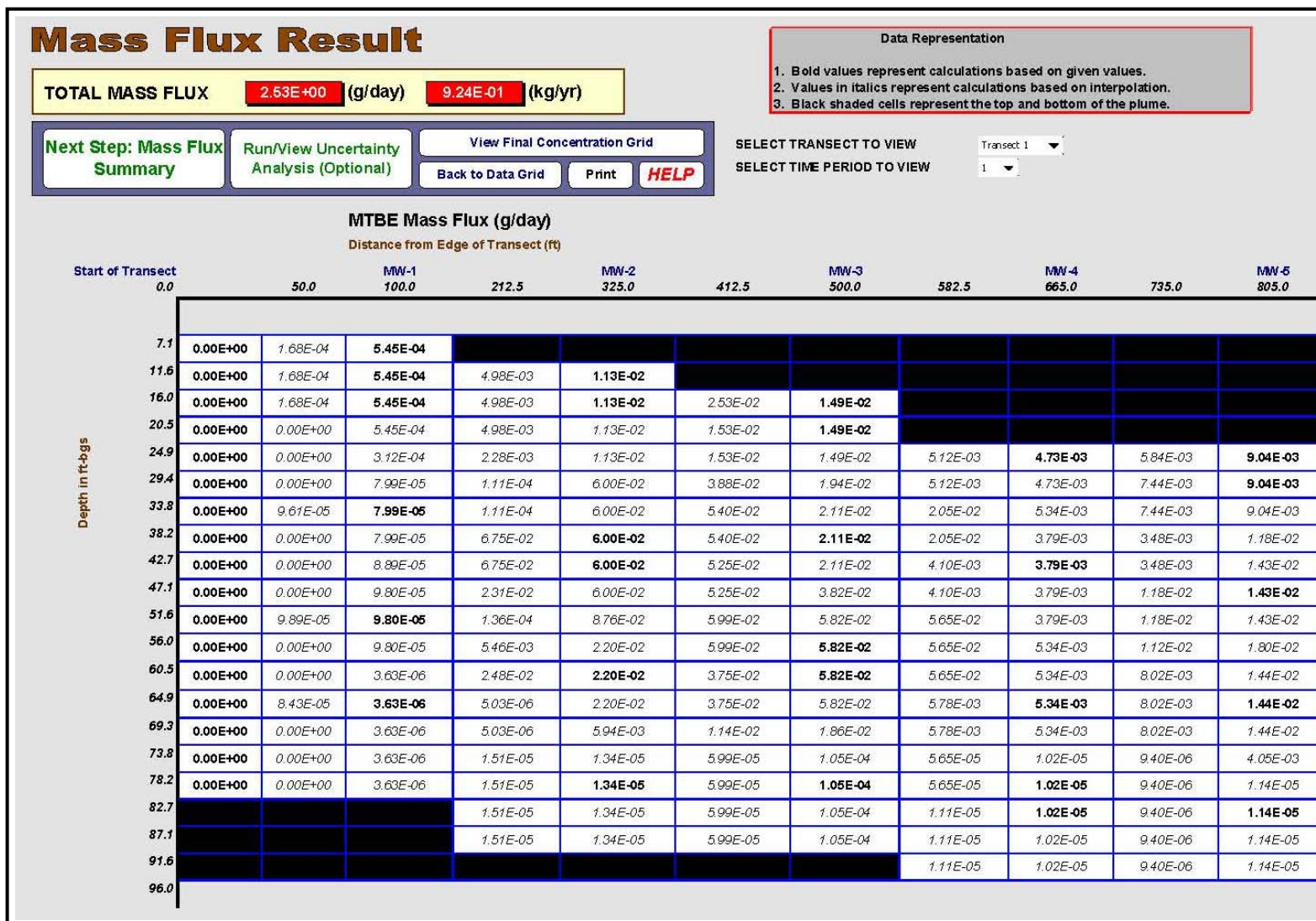


Figure 3-8. MTBE Nearest Neighbor Interpolation: Mass Flux Results Grid – Page 1

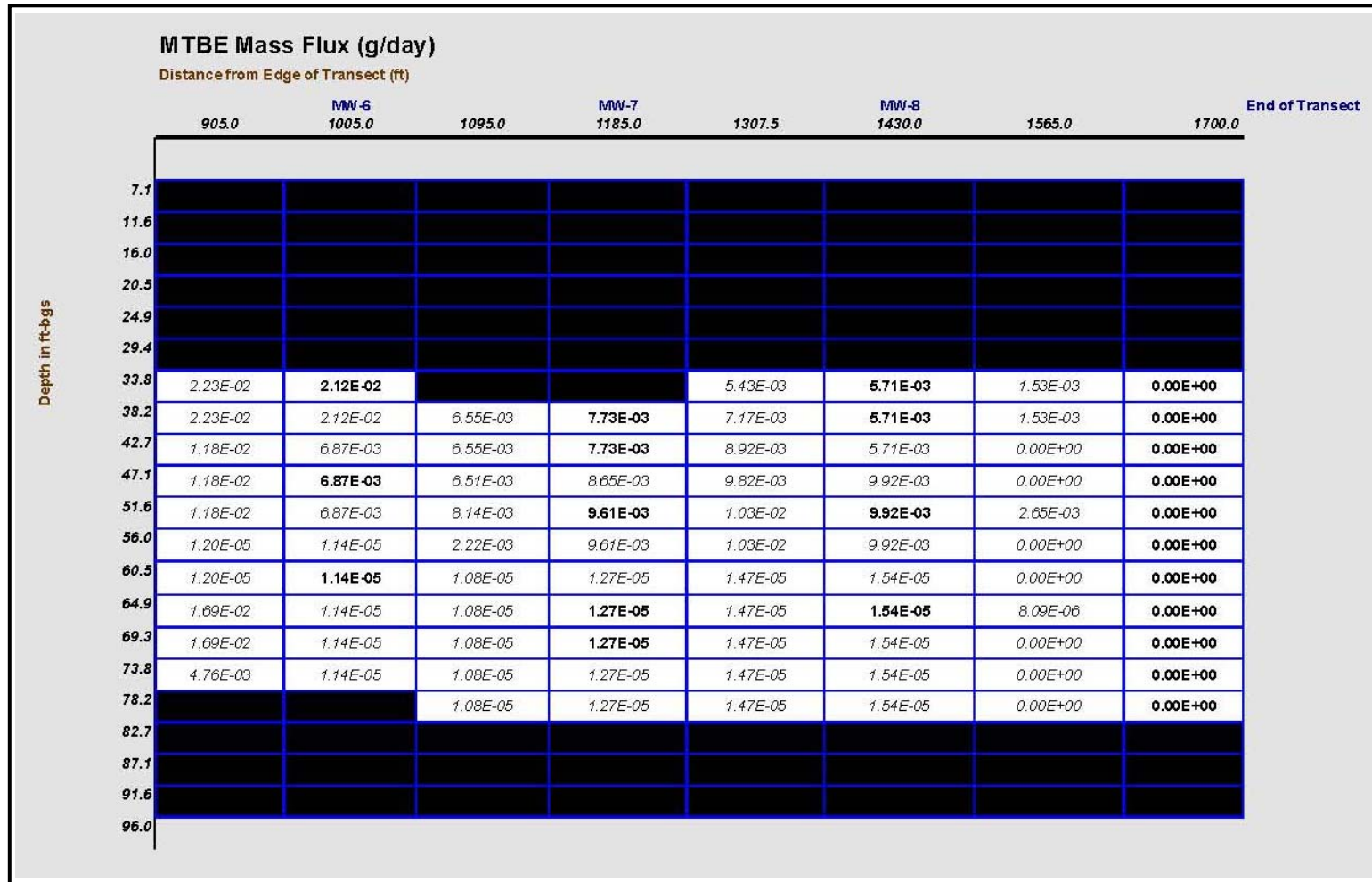


Figure 3-9. MTBE Nearest Neighbor Interpolation: Mass Flux Results Grid – Page 2

CASE STUDY: MTBE AND TBA

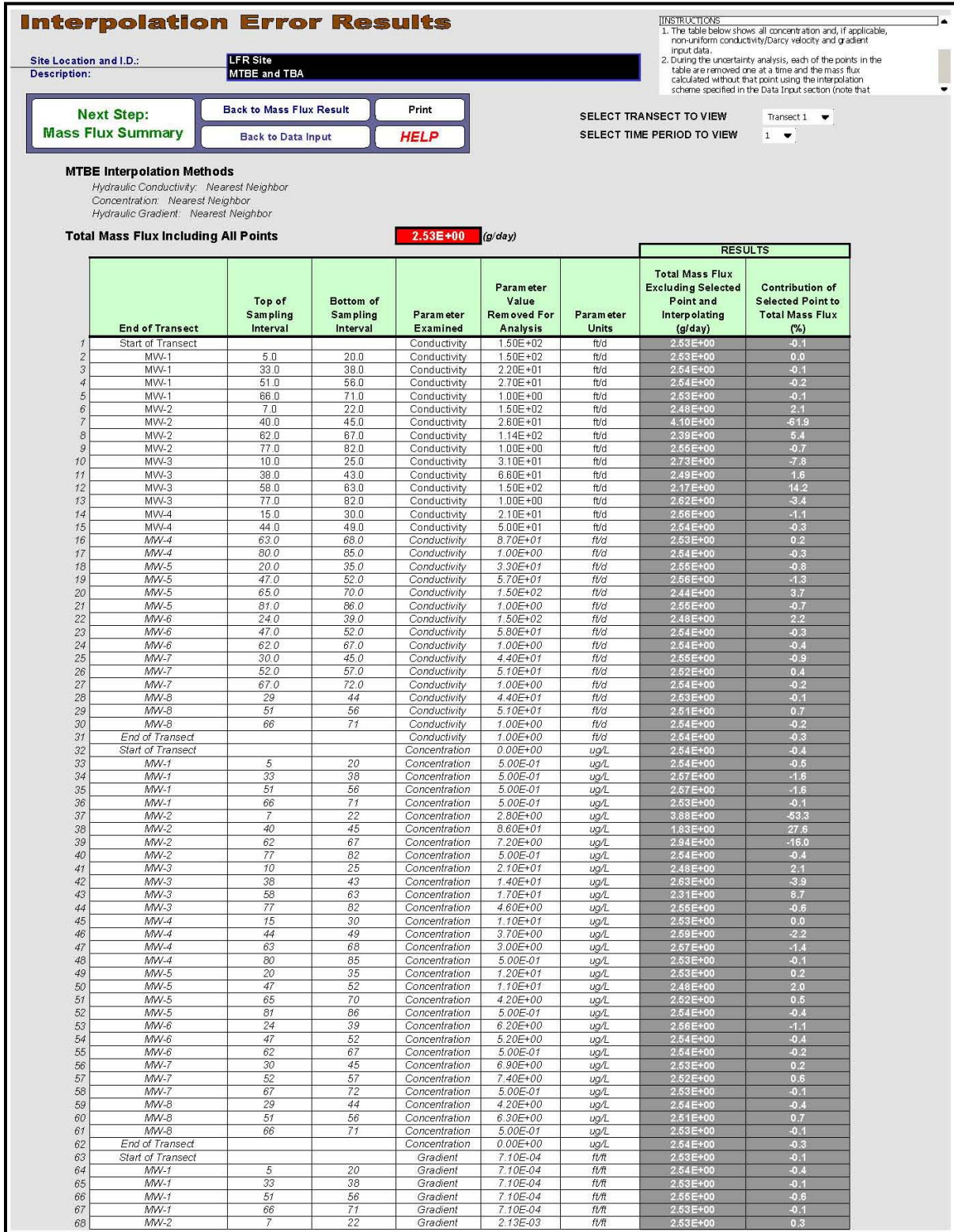


Figure 3-10. MTBE Nearest Neighbor Interpolation: Simple Uncertainty Analysis – Page 1

CASE STUDY: MTBE AND TBA

							RESULTS	
	End of Transect	Top of Sampling Interval	Bottom of Sampling Interval	Parameter Examined	Parameter Value Removed For Analysis	Parameter Units	Total Mass Flux Excluding Selected Point and Interpolating (g/day)	Contribution of Selected Point to Total Mass Flux (%)
69	MW-2	40	45	Gradient	2.13E-03	ft/ft	2.43E+00	3.9
70	MW-2	62	67	Gradient	2.13E-03	ft/ft	2.51E+00	0.7
71	MW-2	77	82	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
72	MW-3	10	25	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
73	MW-3	38	43	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
74	MW-3	58	63	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
75	MW-3	77	82	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
76	MW-4	15	30	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
77	MW-4	44	49	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
78	MW-4	63	68	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
79	MW-4	80	85	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
80	MW-5	20	35	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
81	MW-5	47	52	Gradient	2.13E-03	ft/ft	2.53E+00	0.0
82	MW-5	65	70	Gradient	2.13E-03	ft/ft	2.53E+00	0.1
83	MW-5	81	86	Gradient	2.13E-03	ft/ft	2.53E+00	-0.1
84	MW-6	24	39	Gradient	1.91E-03	ft/ft	2.54E+00	-0.2
85	MW-6	47	52	Gradient	1.91E-03	ft/ft	2.54E+00	-0.1
86	MW-6	62	67	Gradient	1.91E-03	ft/ft	2.53E+00	-0.1
87	MW-7	30	45	Gradient	1.91E-03	ft/ft	2.53E+00	-0.1
88	MW-7	52	57	Gradient	1.91E-03	ft/ft	2.53E+00	-0.1
89	MW-7	67	72	Gradient	1.91E-03	ft/ft	2.53E+00	-0.1
90	MW-8	29	44	Gradient	1.91E-03	ft/ft	2.53E+00	-0.1
91	MW-8	51	56	Gradient	1.91E-03	ft/ft	2.53E+00	-0.1
92	MW-8	66	71	Gradient	1.91E-03	ft/ft	2.53E+00	-0.1
93	End of Transect			Gradient	1.91E-03	ft/ft	2.53E+00	-0.1

Figure 3-11. MTBE Nearest Neighbor Interpolation: Simple Uncertainty Analysis – Page 2

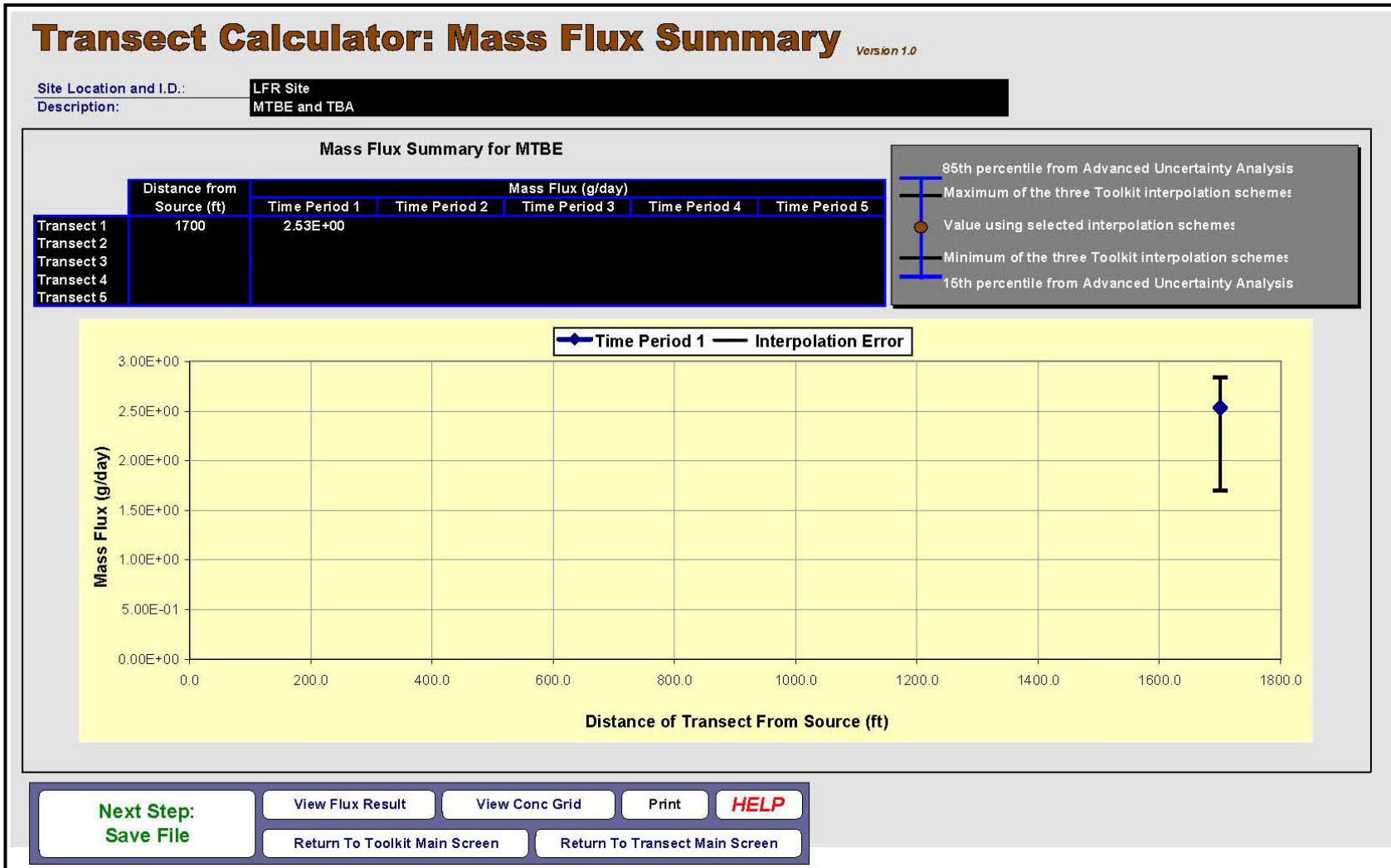


Figure 3-12. MTBE Nearest Neighbor Interpolation: Mass Flux Summary

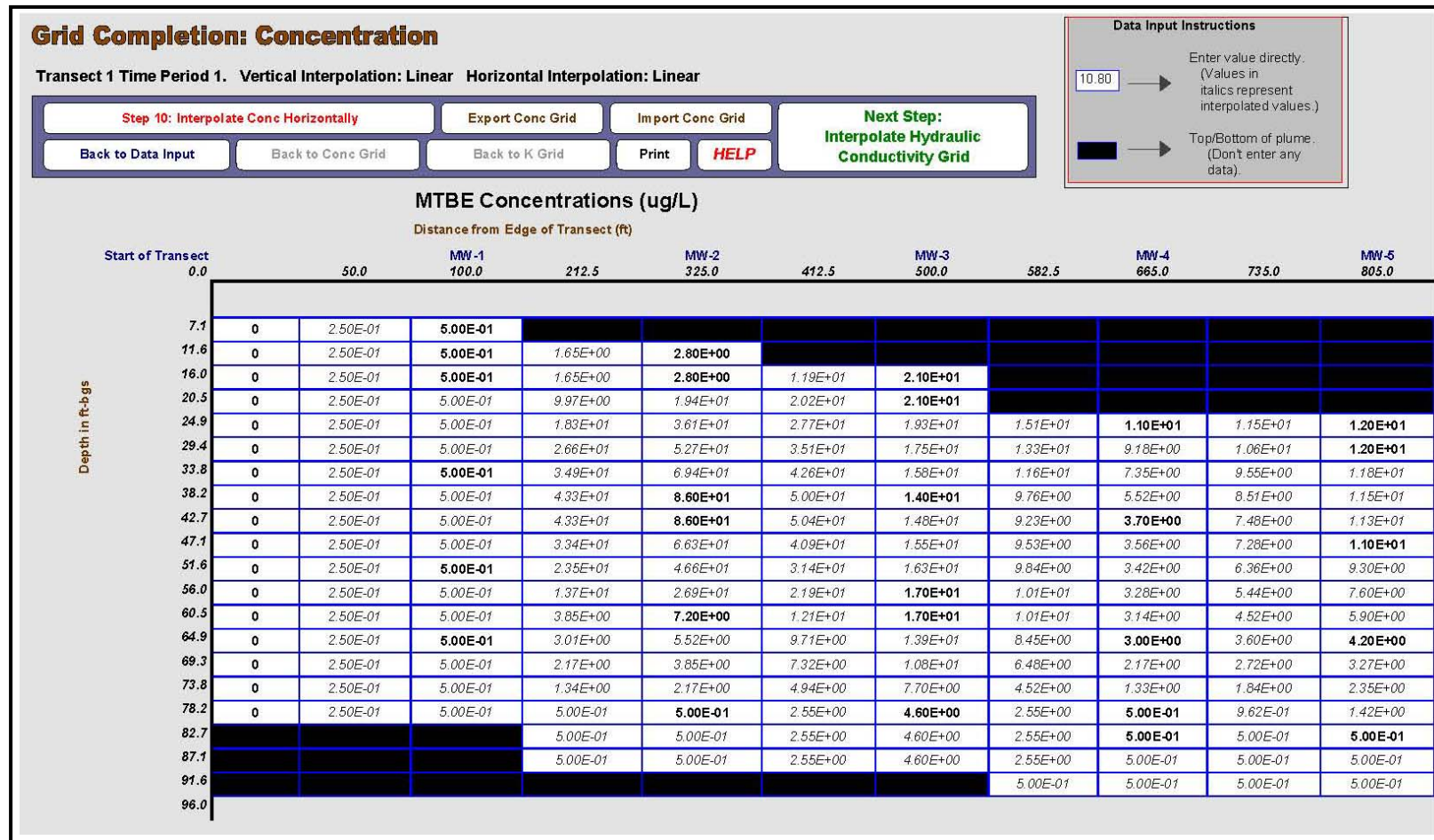


Figure 3-13. MTBE Linear Interpolation: Concentration Grid – Page 1

CASE STUDY: MTBE AND TBA

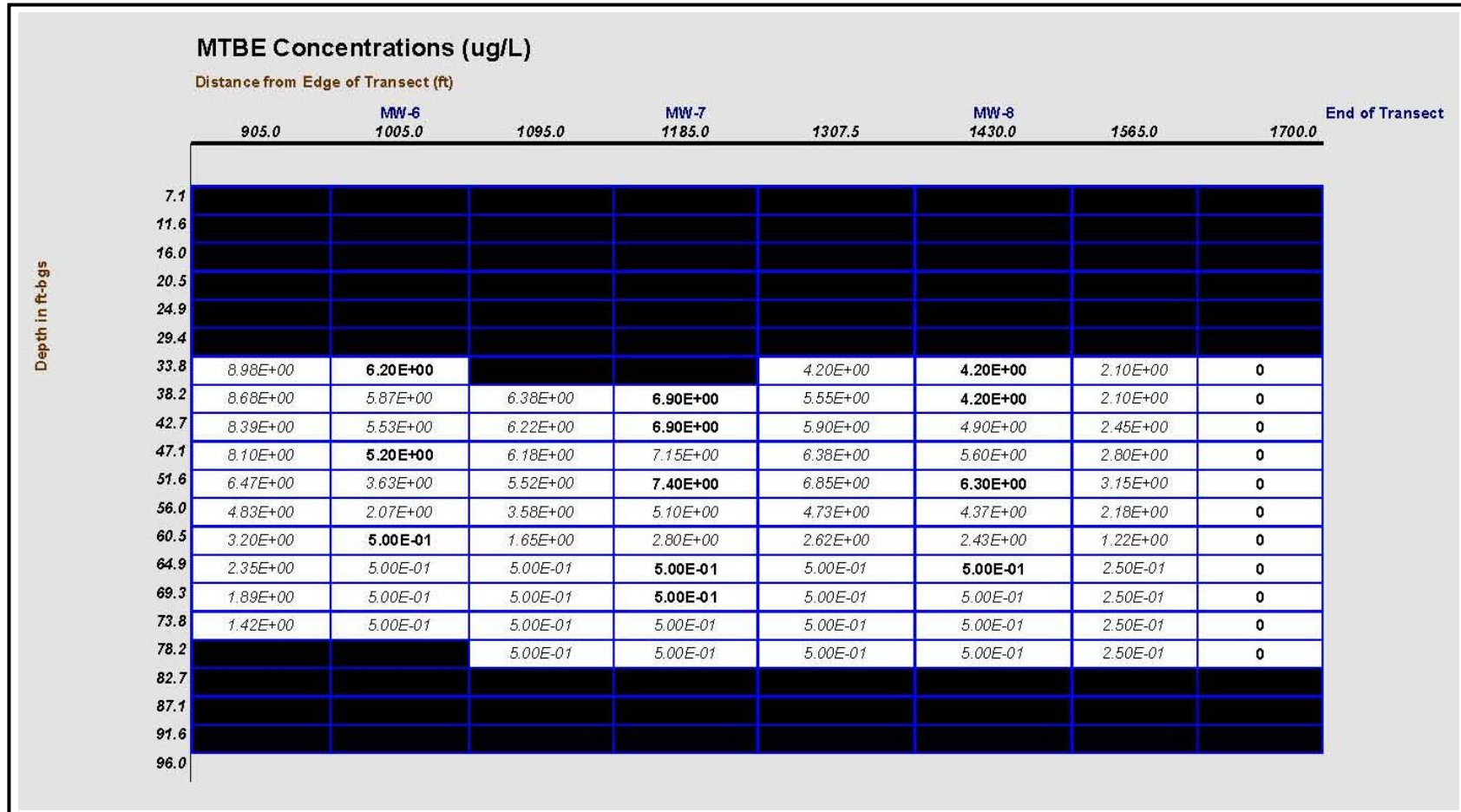


Figure 3-14. MTBE Linear Interpolation: Concentration Grid – Page 2

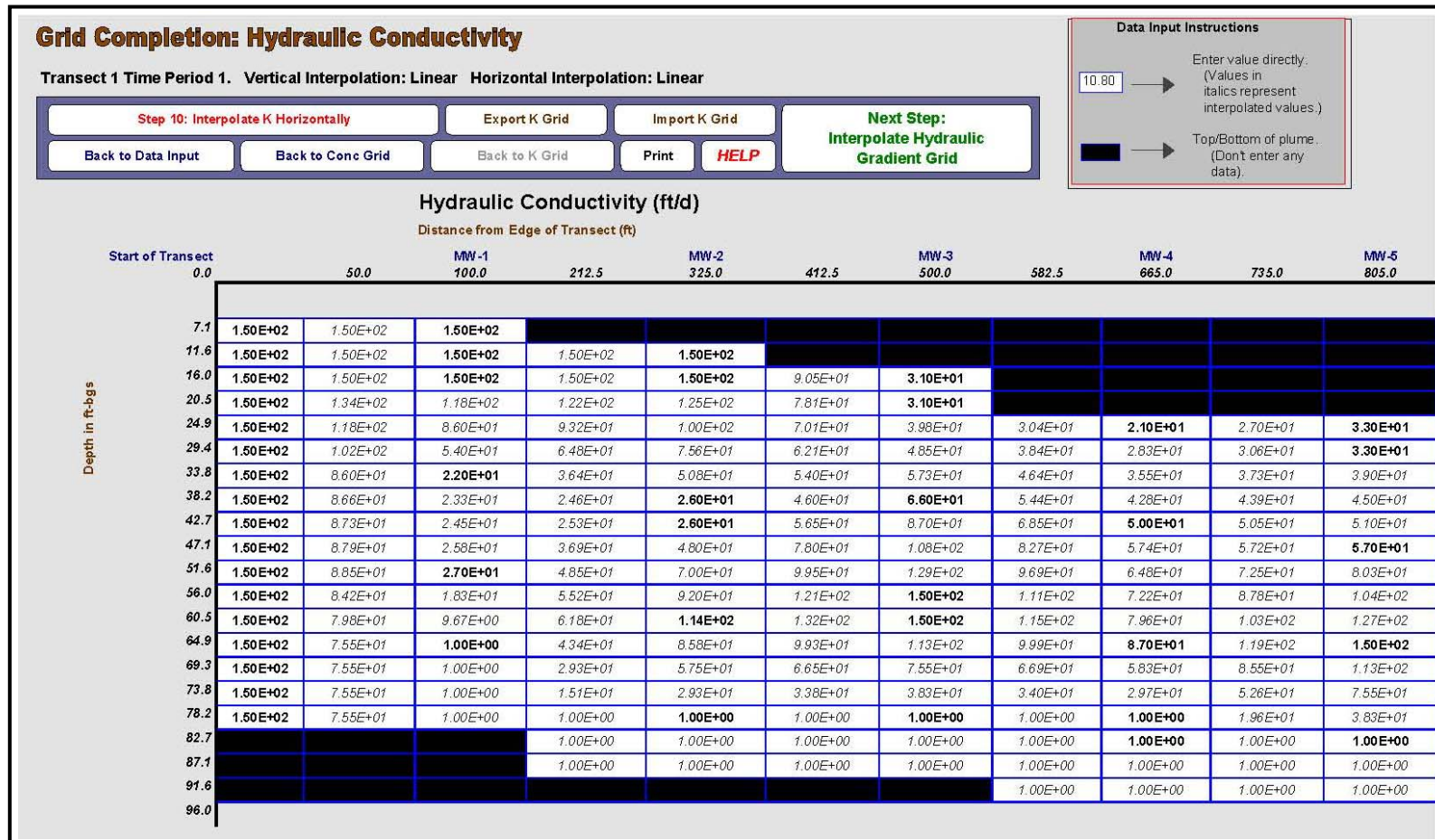


Figure 3-15. Linear Interpolation: Hydraulic Conductivity Grid – Page 1

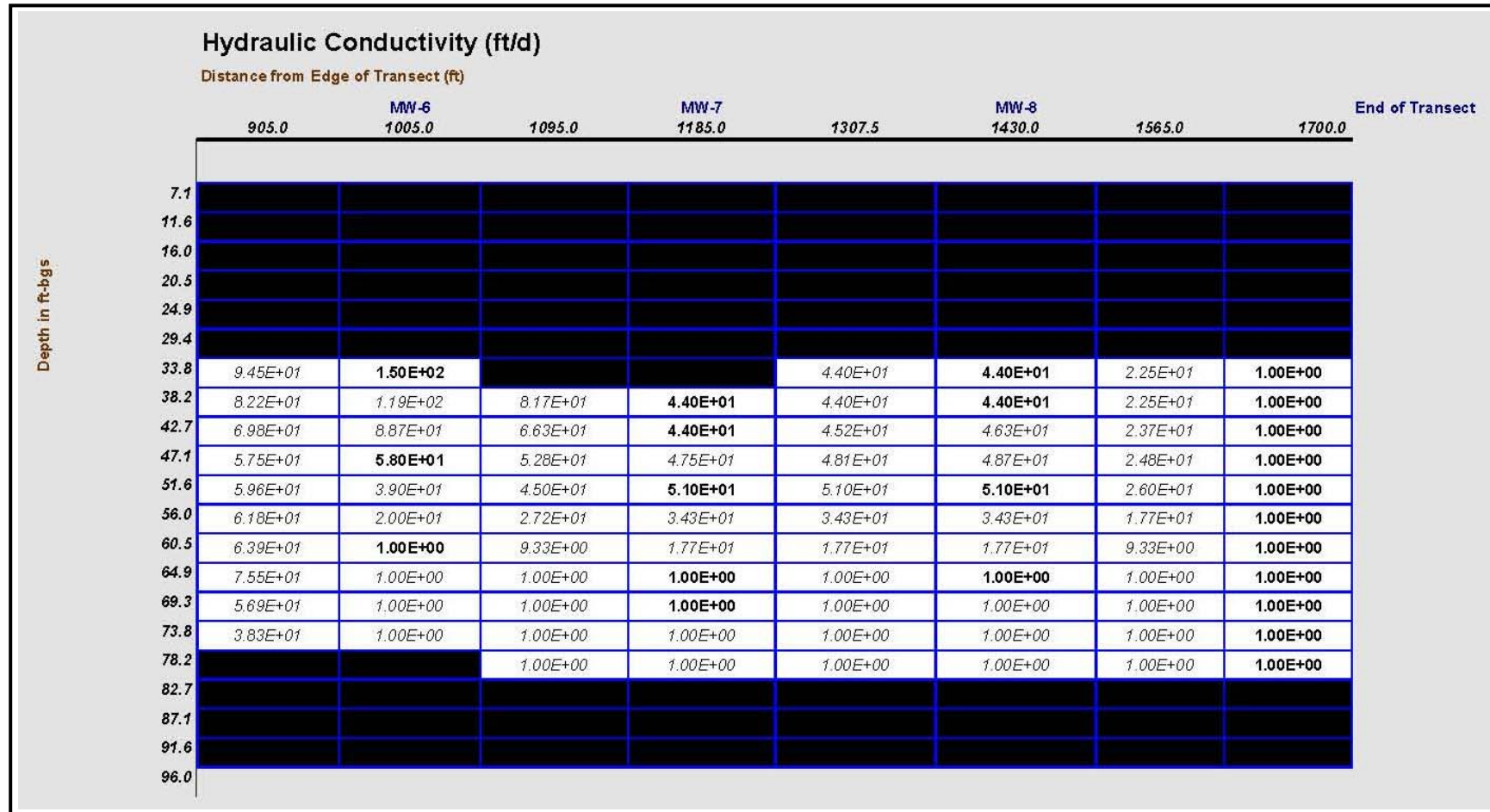


Figure 3-16. Linear Interpolation: Hydraulic Conductivity Grid – Page 2

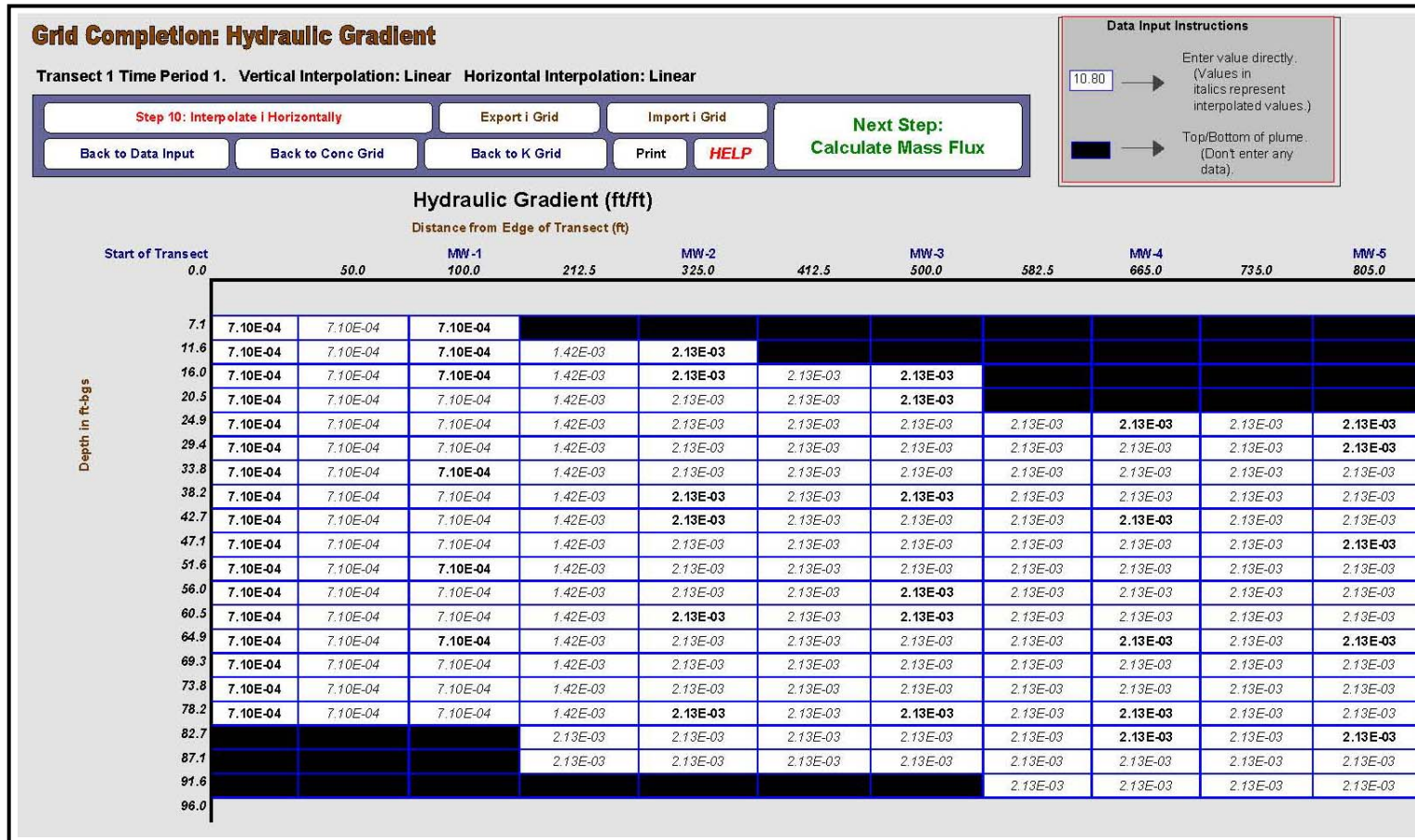


Figure 3-17. Linear Interpolation: Hydraulic Gradient Grid – Page 1

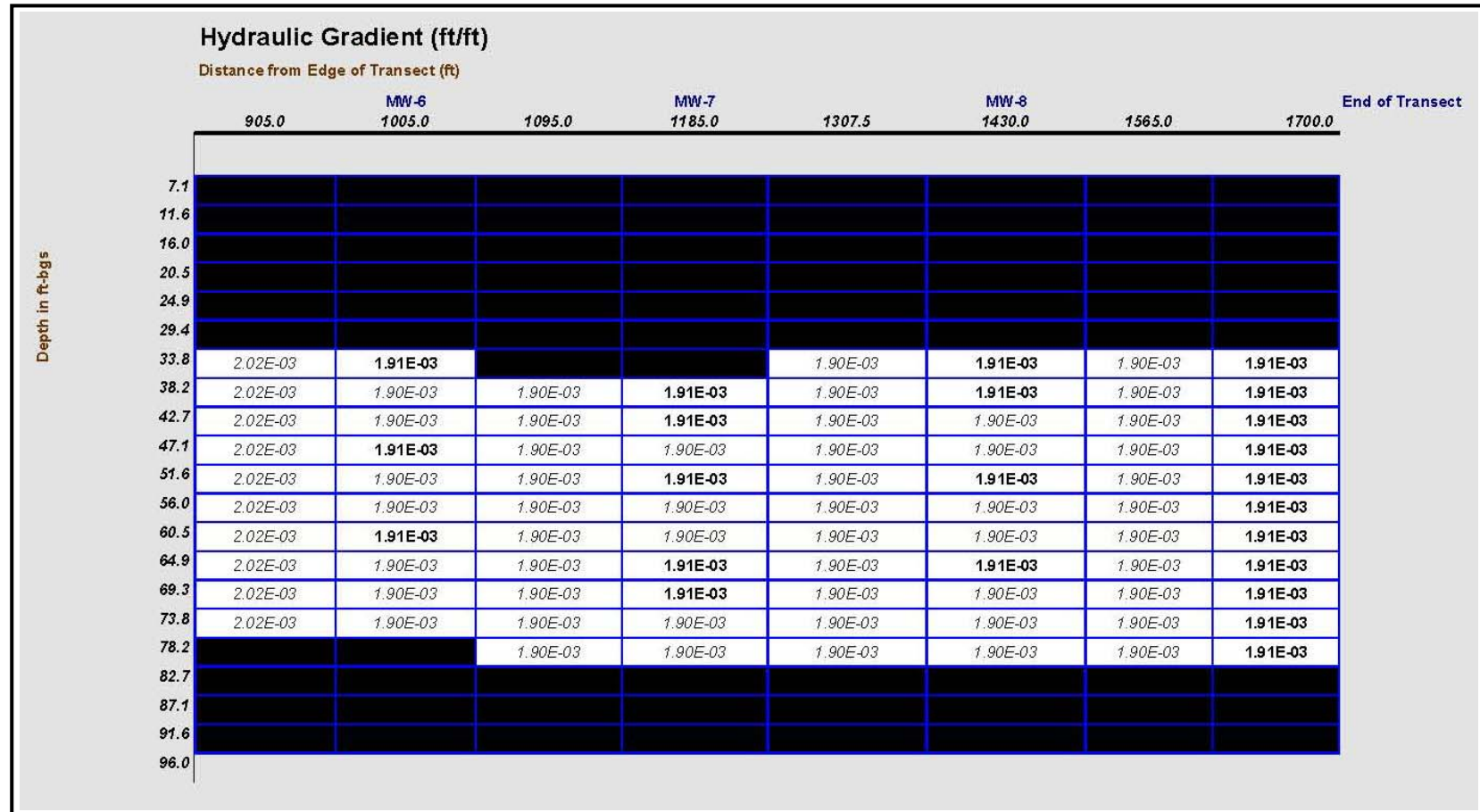


Figure 3-18. Linear Interpolation: Hydraulic Gradient Grid – Page 2

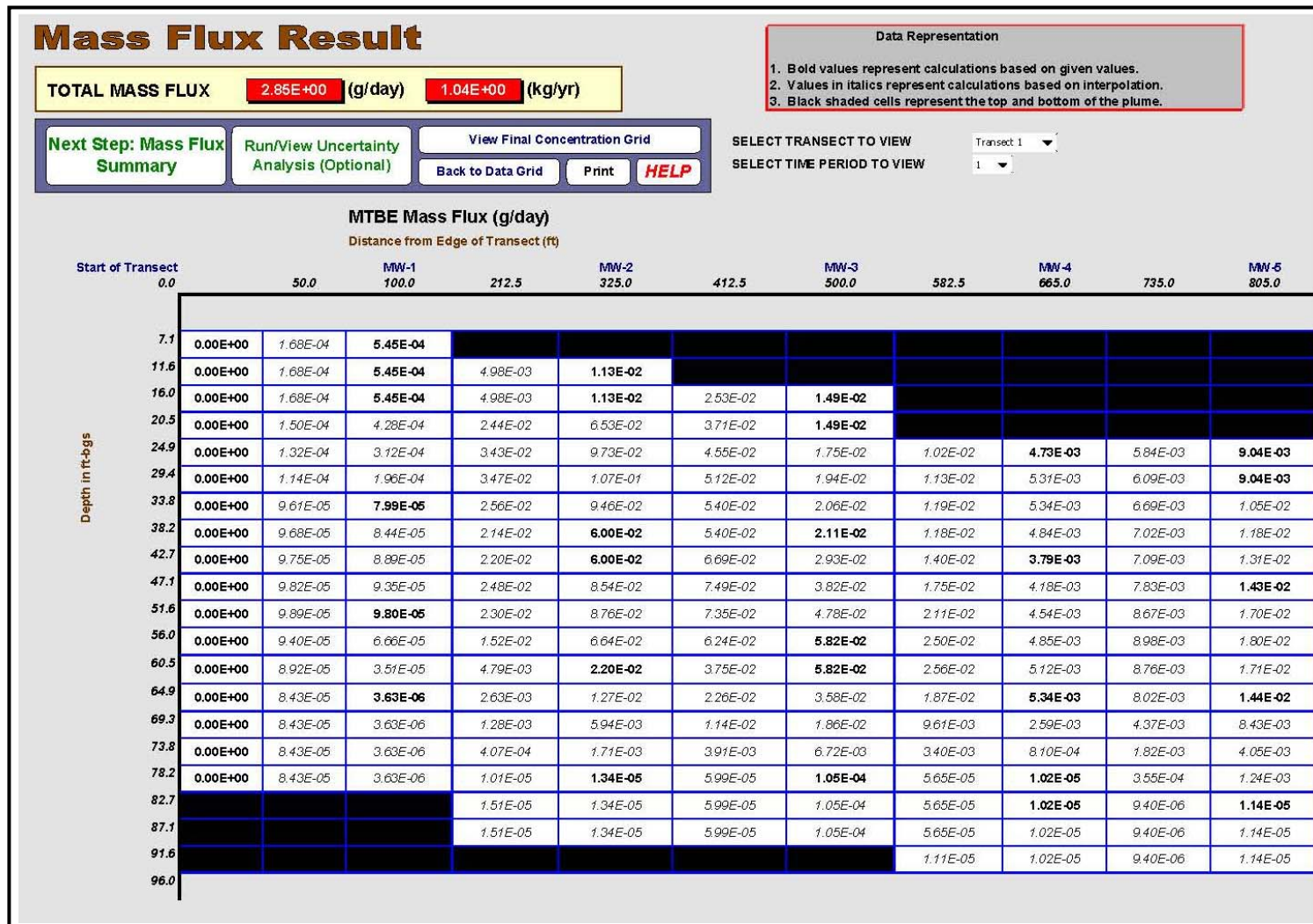


Figure 3-19. MTBE Linear Interpolation: Mass Flux Results Grid – Page 1

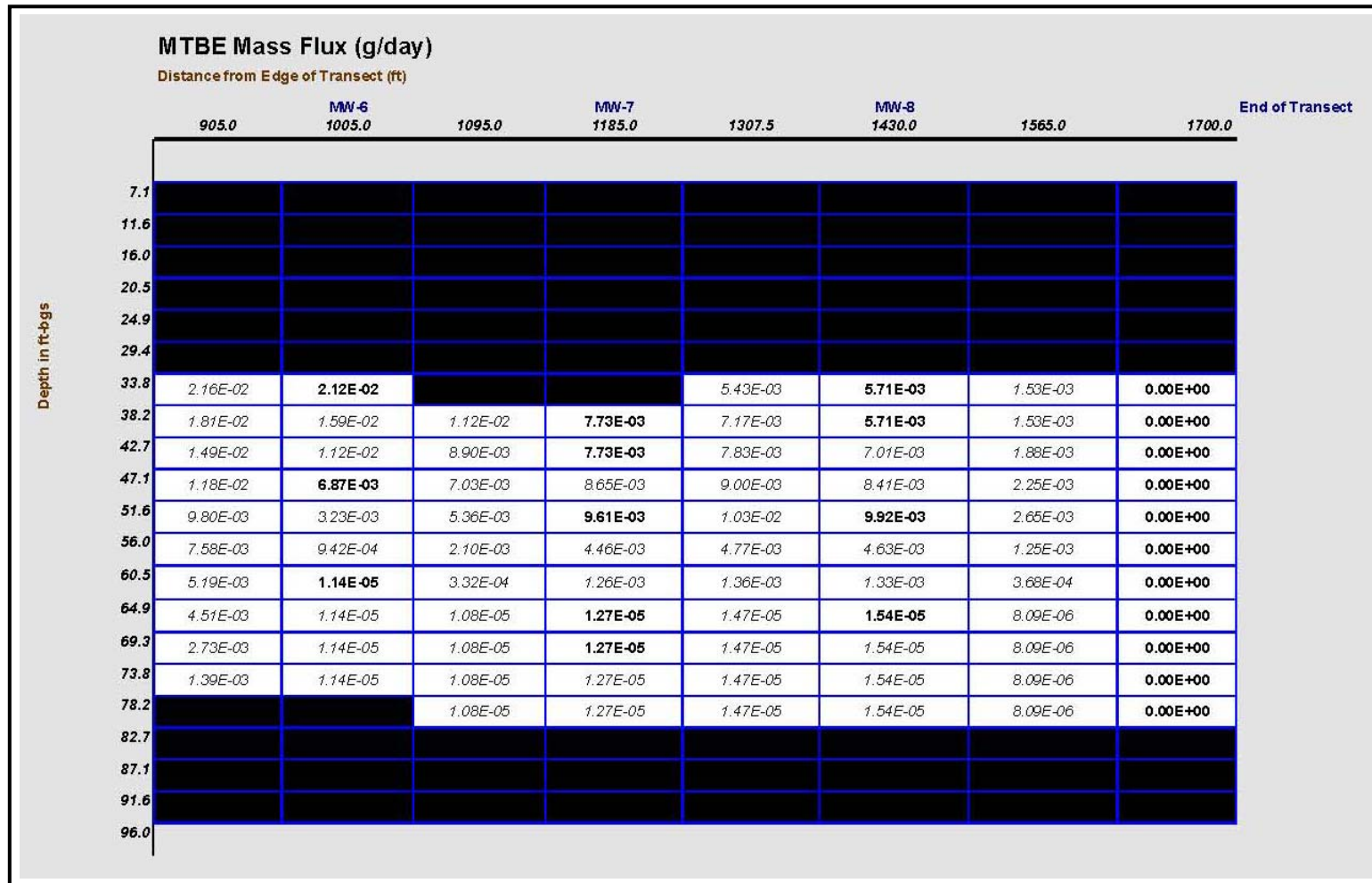


Figure 3-20. MTBE Linear Interpolation: Mass Flux Results Grid – Page 2

CASE STUDY: MTBE AND TBA

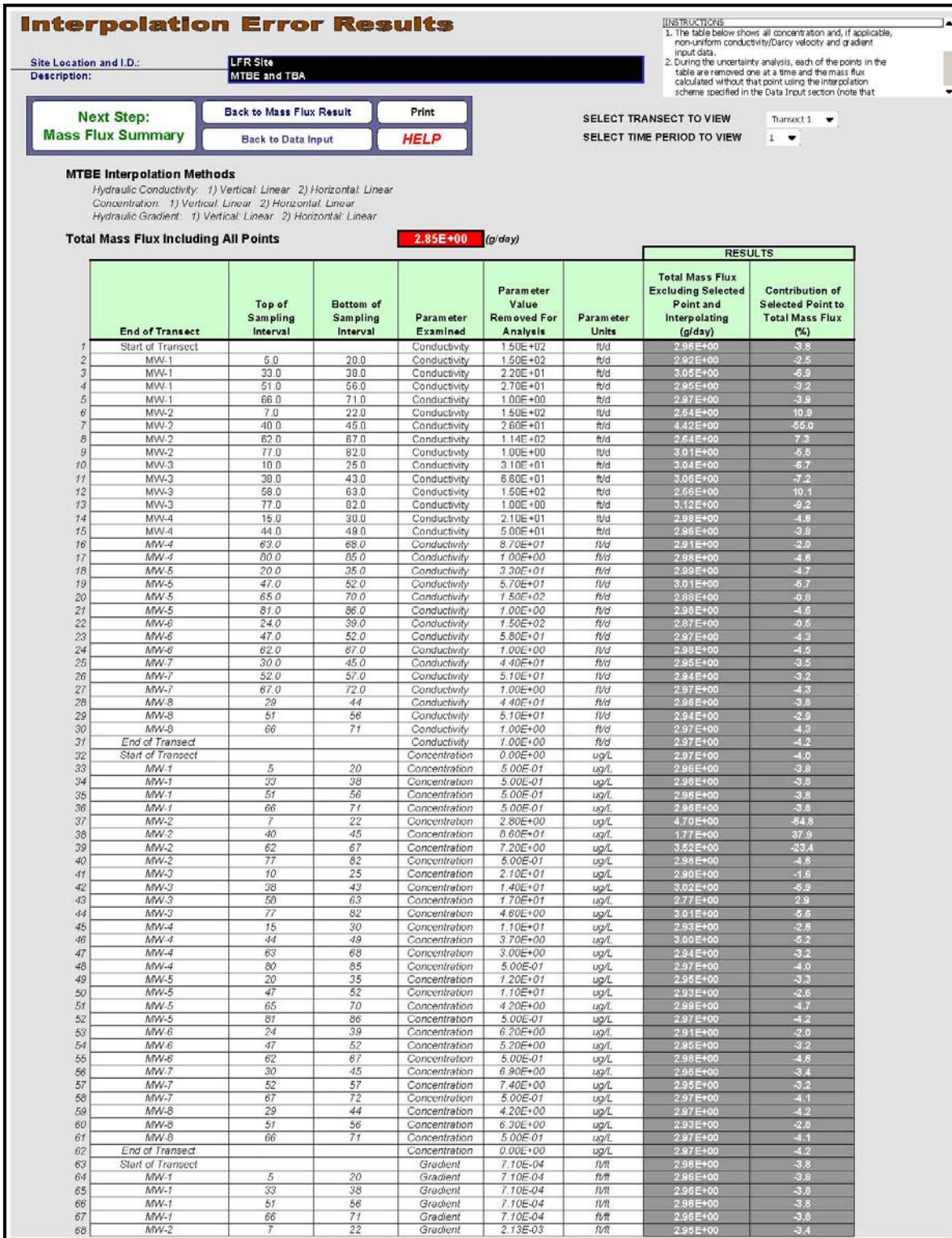


Figure 3-21. MTBE Linear Interpolation: Simple Uncertainty Analysis – Page 1

CASE STUDY: MTBE AND TBA

						RESULTS		
	End of Transect	Top of Sampling Interval	Bottom of Sampling Interval	Parameter Examined	Parameter Value Removed For Analysis	Parameter Units	Total Mass Flux Excluding Selected Point and Interpolating (g/day)	Contribution of Selected Point to Total Mass Flux (%)
69	MW-2	40	45	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
70	MW-2	62	67	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
71	MW-2	77	82	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
72	MW-3	10	25	Gradient	2.13E-03	ft/ft	2.95E+00	-3.3
73	MW-3	38	43	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
74	MW-3	58	63	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
75	MW-3	77	82	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
76	MW-4	15	30	Gradient	2.13E-03	ft/ft	2.95E+00	-3.5
77	MW-4	44	49	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
78	MW-4	63	68	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
79	MW-4	80	85	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
80	MW-5	20	35	Gradient	2.13E-03	ft/ft	2.95E+00	-3.5
81	MW-5	47	52	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
82	MW-5	65	70	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
83	MW-5	81	86	Gradient	2.13E-03	ft/ft	2.96E+00	-3.8
84	MW-6	24	39	Gradient	1.91E-03	ft/ft	2.92E+00	-2.3
85	MW-6	47	52	Gradient	1.91E-03	ft/ft	2.96E+00	-3.8
86	MW-6	62	67	Gradient	1.91E-03	ft/ft	2.96E+00	-3.8
87	MW-7	30	45	Gradient	1.91E-03	ft/ft	2.95E+00	-3.2
88	MW-7	52	57	Gradient	1.91E-03	ft/ft	2.96E+00	-3.8
89	MW-7	67	72	Gradient	1.91E-03	ft/ft	2.96E+00	-3.8
90	MW-8	29	44	Gradient	1.91E-03	ft/ft	2.96E+00	-3.6
91	MW-8	51	56	Gradient	1.91E-03	ft/ft	2.96E+00	-3.8
92	MW-8	66	71	Gradient	1.91E-03	ft/ft	2.96E+00	-3.8
93	End of Transect			Gradient	1.91E-03	ft/ft	2.96E+00	-3.8

Figure 3-22. MTBE Linear Interpolation: Simple Uncertainty Analysis – Page 2

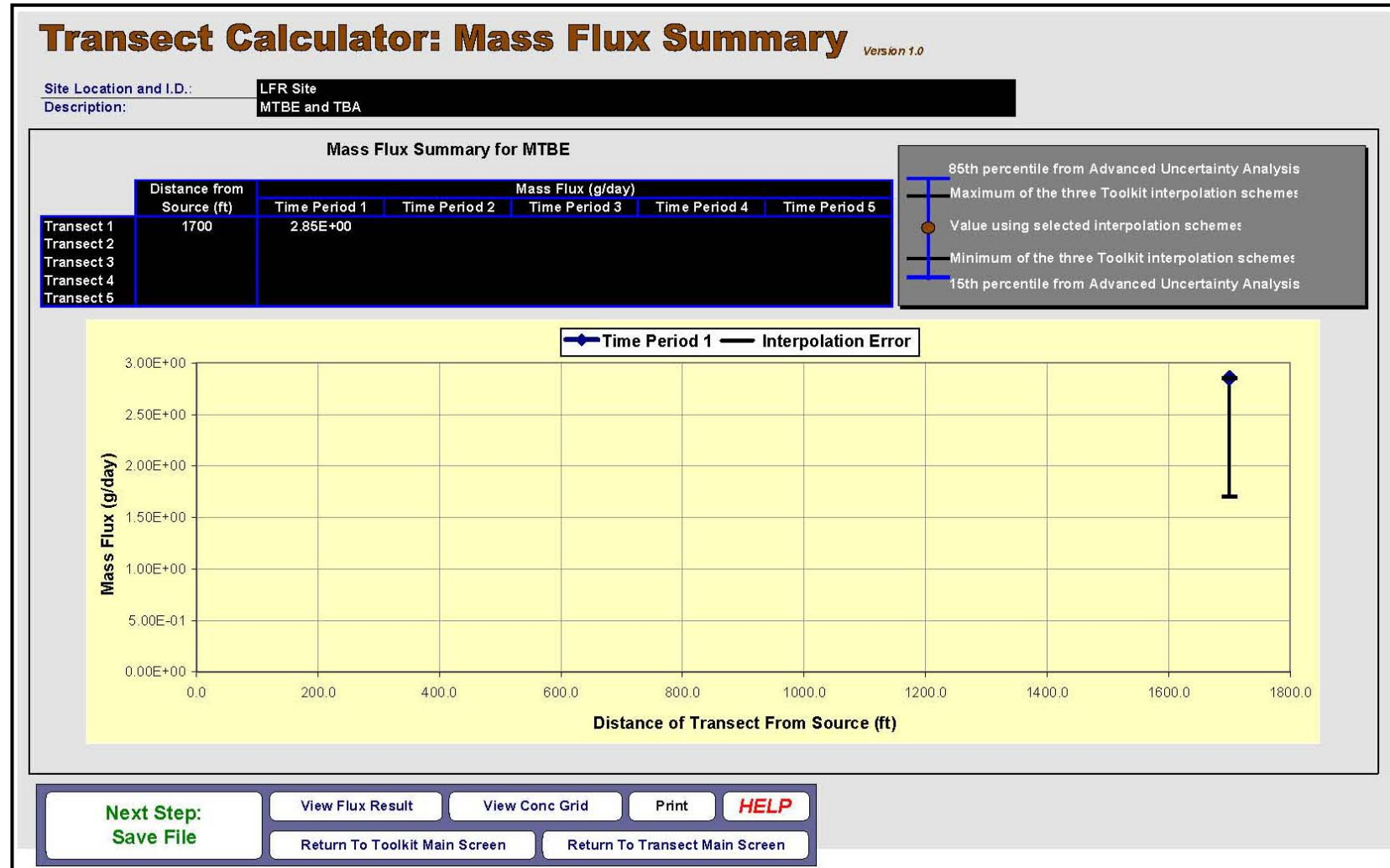


Figure 3-23. MTBE Linear Interpolation: Mass Flux Summary

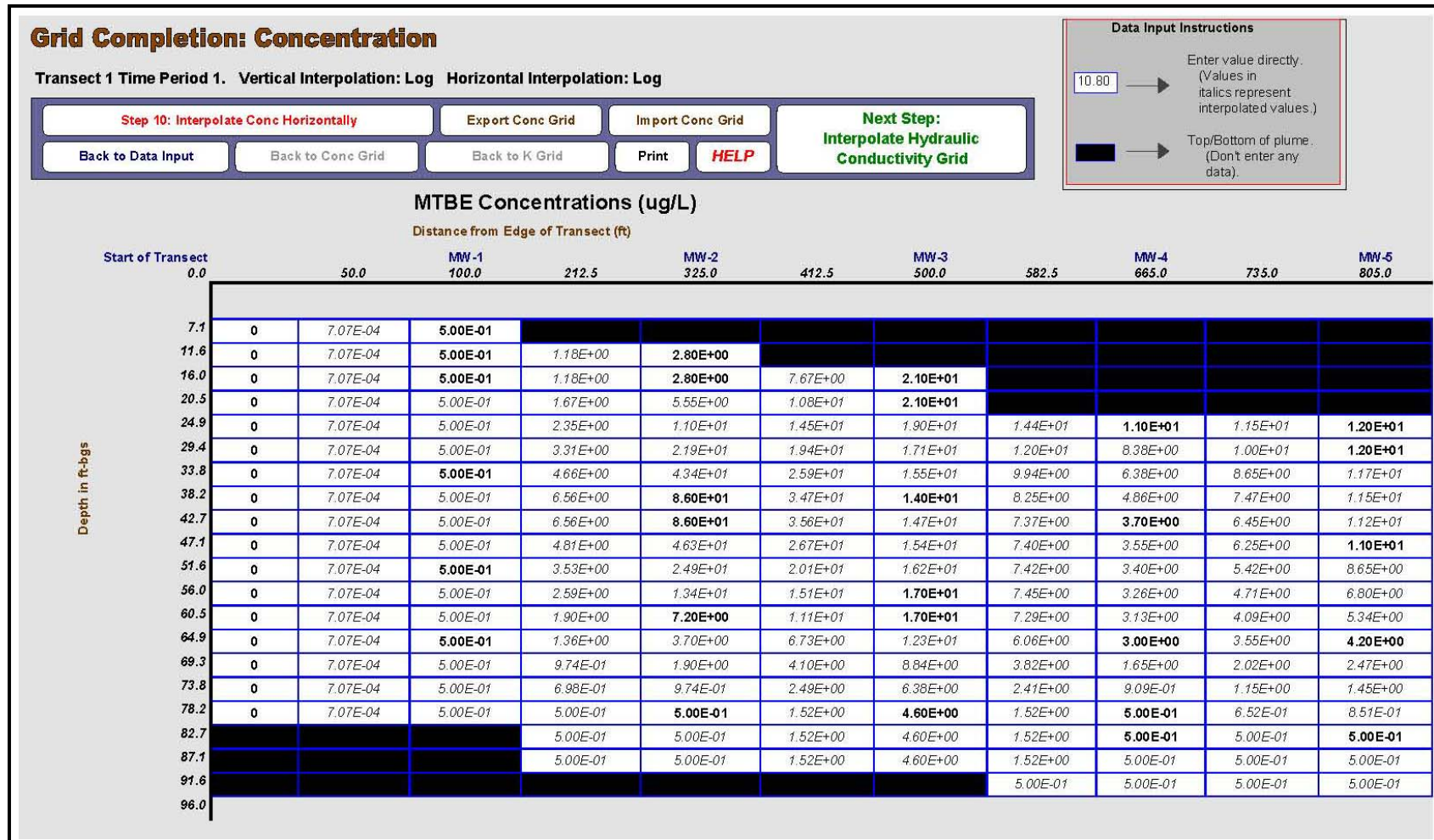


Figure 3-24. MTBE Log Transformation: Concentration Grid – Page 1

CASE STUDY: MTBE AND TBA

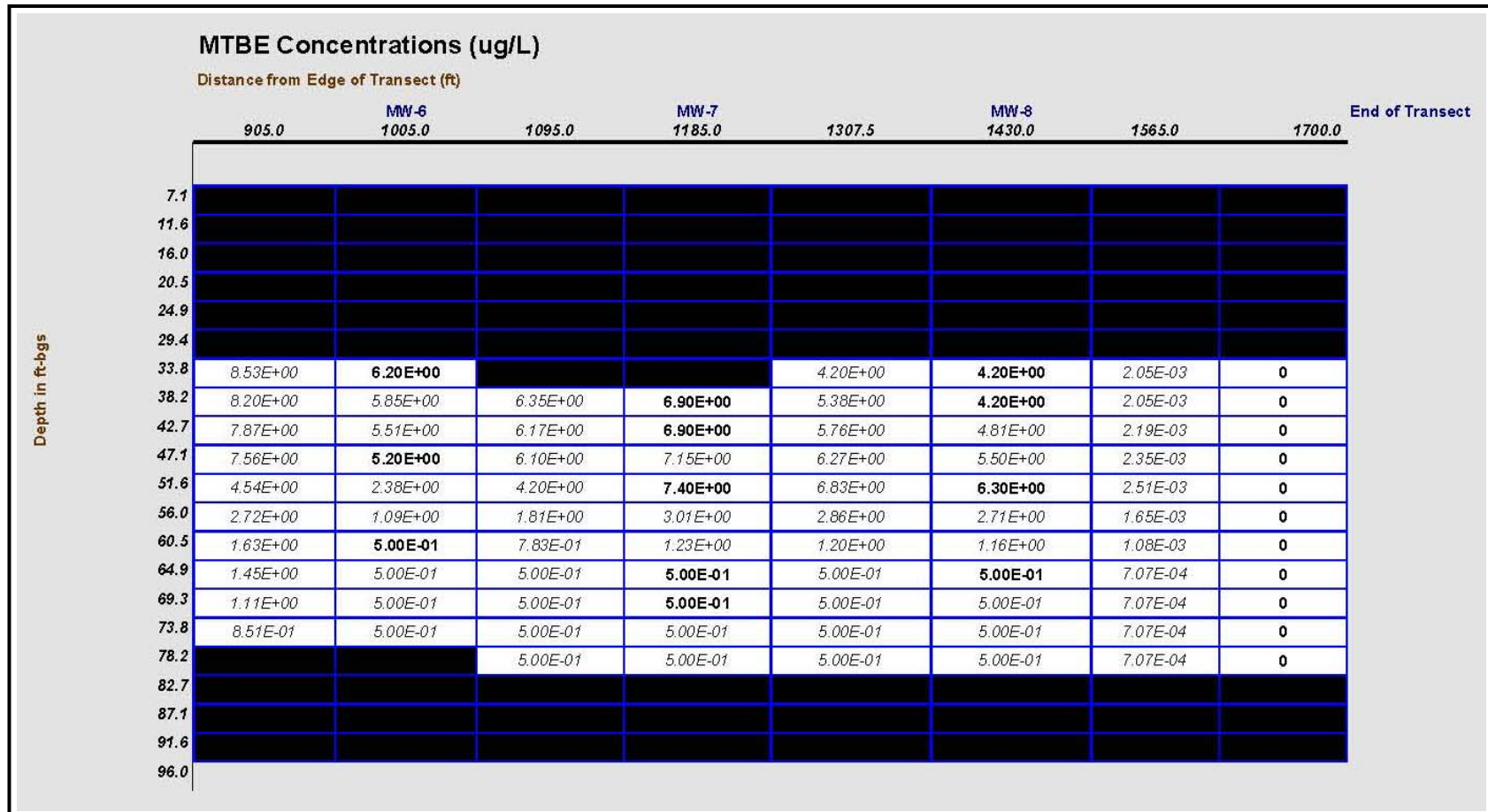


Figure 3-25. MTBE Log Transformation: Concentration Grid – Page 2

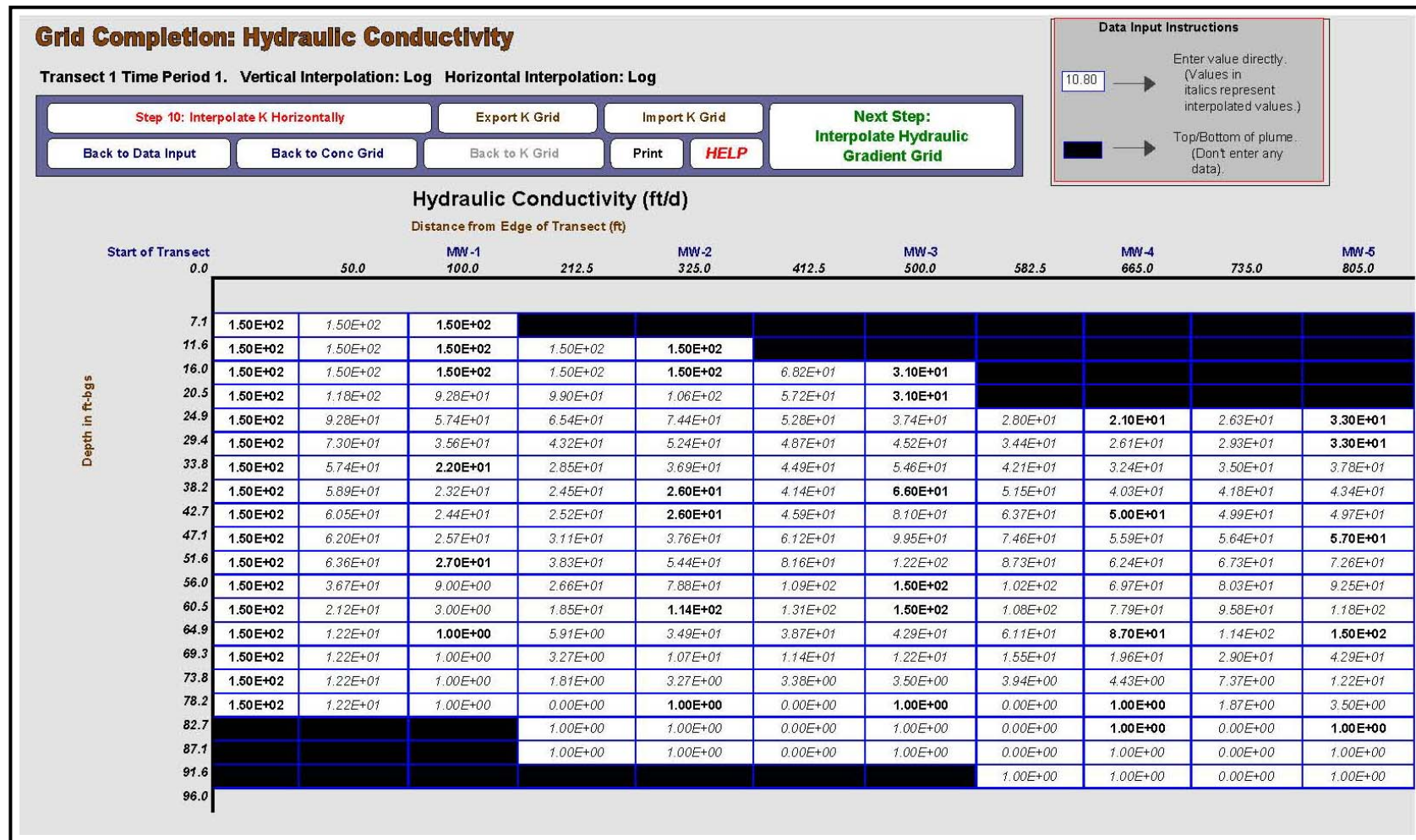


Figure 3-26. Log Transformation: Hydraulic Conductivity Grid – Page 1

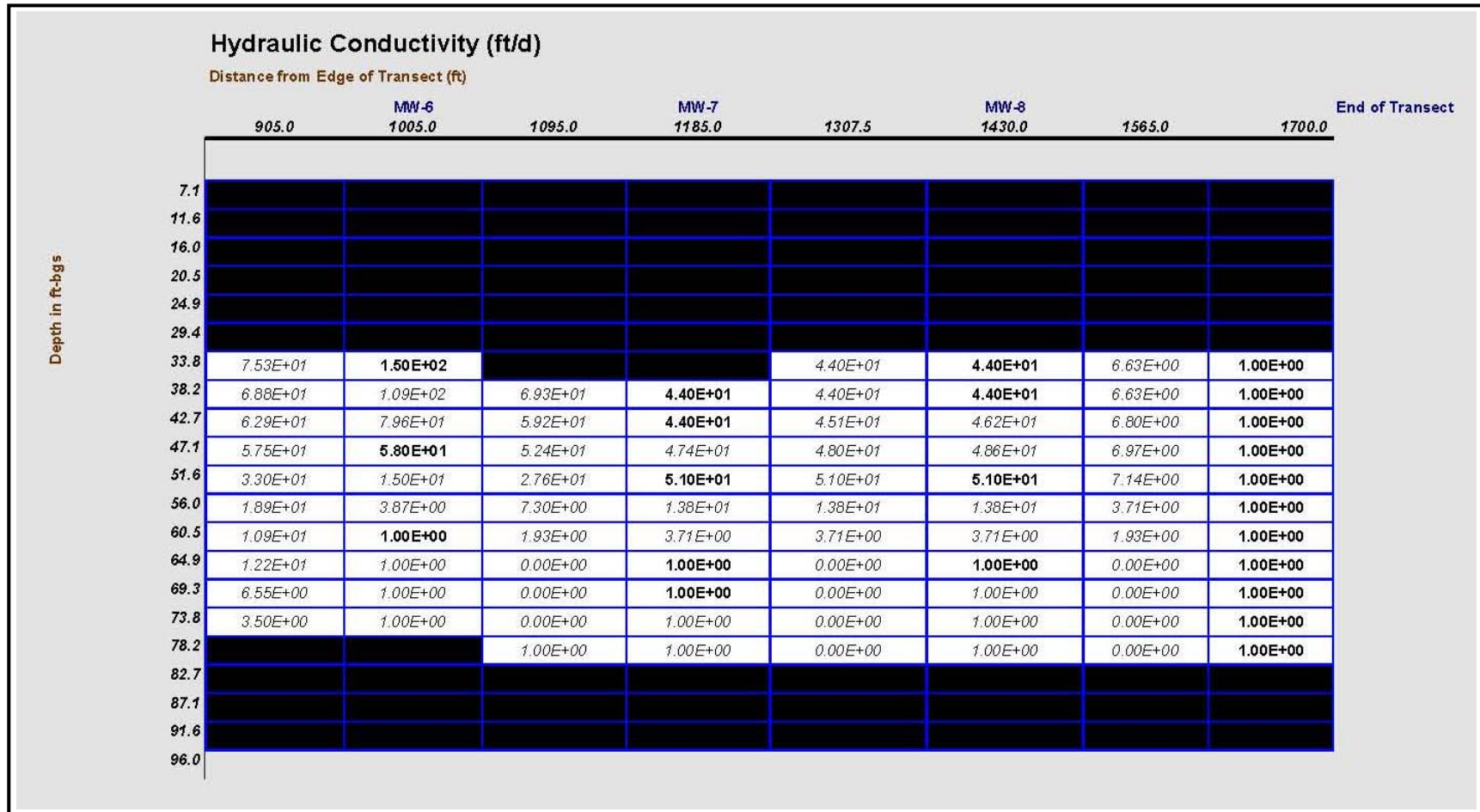


Figure 3-27. Log Transformation: Hydraulic Conductivity Grid – Page 2

Grid Completion: Hydraulic Gradient

Transect 1 Time Period 1. Vertical Interpolation: Log Horizontal Interpolation: Log

Step 10: Interpolate i Horizontally Export i Grid Import i Grid **Next Step: Calculate Mass Flux**

Back to Data Input Back to Conc Grid Back to K Grid Print **HELP**

Hydraulic Gradient (ft/ft)

Distance from Edge of Transect (ft)

Start of Transect	50.0	MW-1 100.0	212.5	MW-2 325.0	412.5	MW-3 500.0	582.5	MW-4 665.0	735.0	MW-5 805.0
7.1	7.10E-04	7.10E-04	7.10E-04							
11.6	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03					
16.0	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03			
20.5	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03			
24.9	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
29.4	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
33.8	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
38.2	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
42.7	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
47.1	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
51.6	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
56.0	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
60.5	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
64.9	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
69.3	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
73.8	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
78.2	7.10E-04	7.10E-04	7.10E-04	1.23E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
82.7				2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
87.1				2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
91.6							2.13E-03	2.13E-03	2.13E-03	2.13E-03
96.0										

Depth in ft-bgs

Data Input Instructions

10.80 → Enter value directly. (Values in italics represent interpolated values.)

■ → Top/Bottom of plume. (Don't enter any data).

Figure 3-28. Log Transformation: Hydraulic Gradient Grid – Page 1

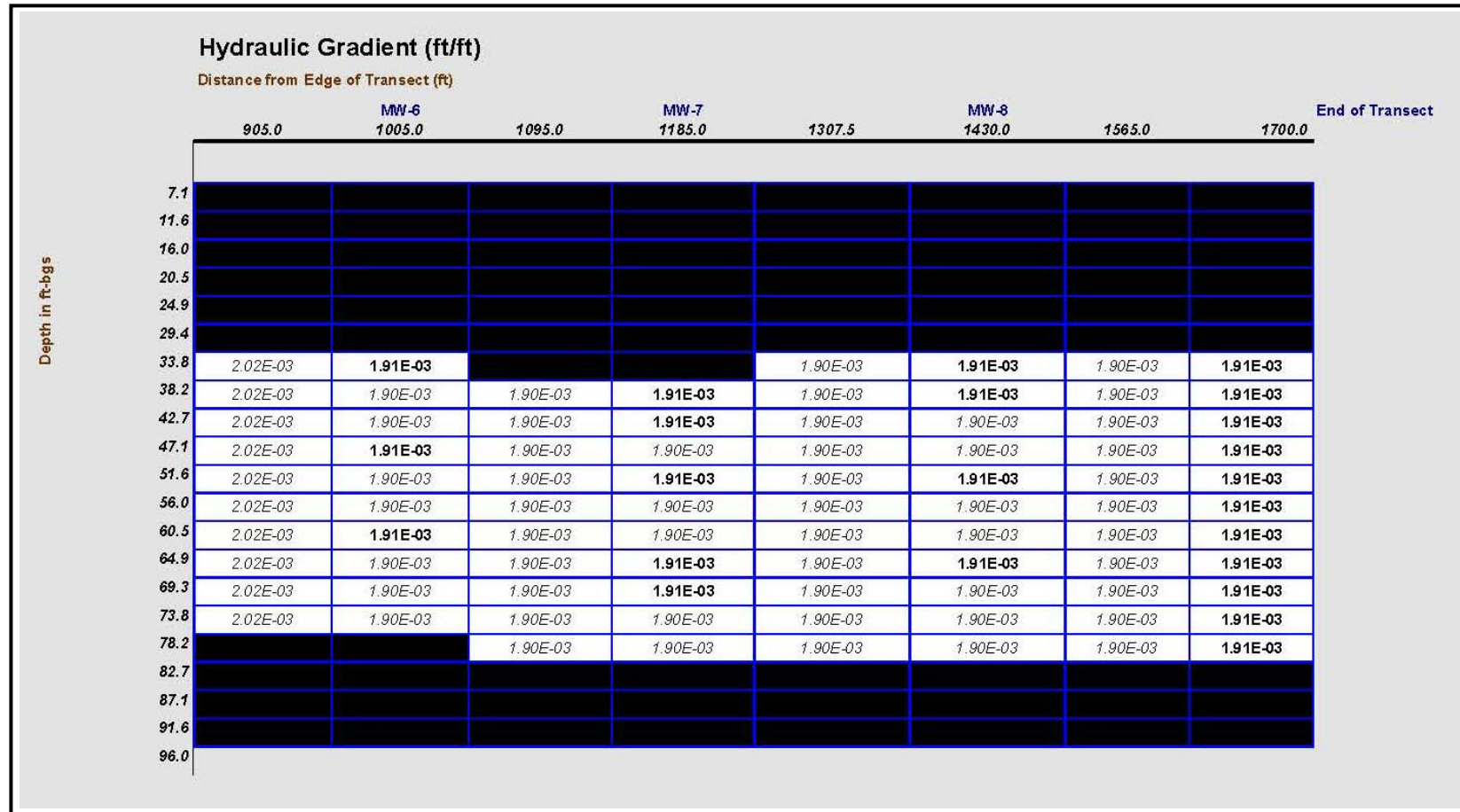


Figure 3-29. Log Transformation: Hydraulic Gradient Grid – Page 2

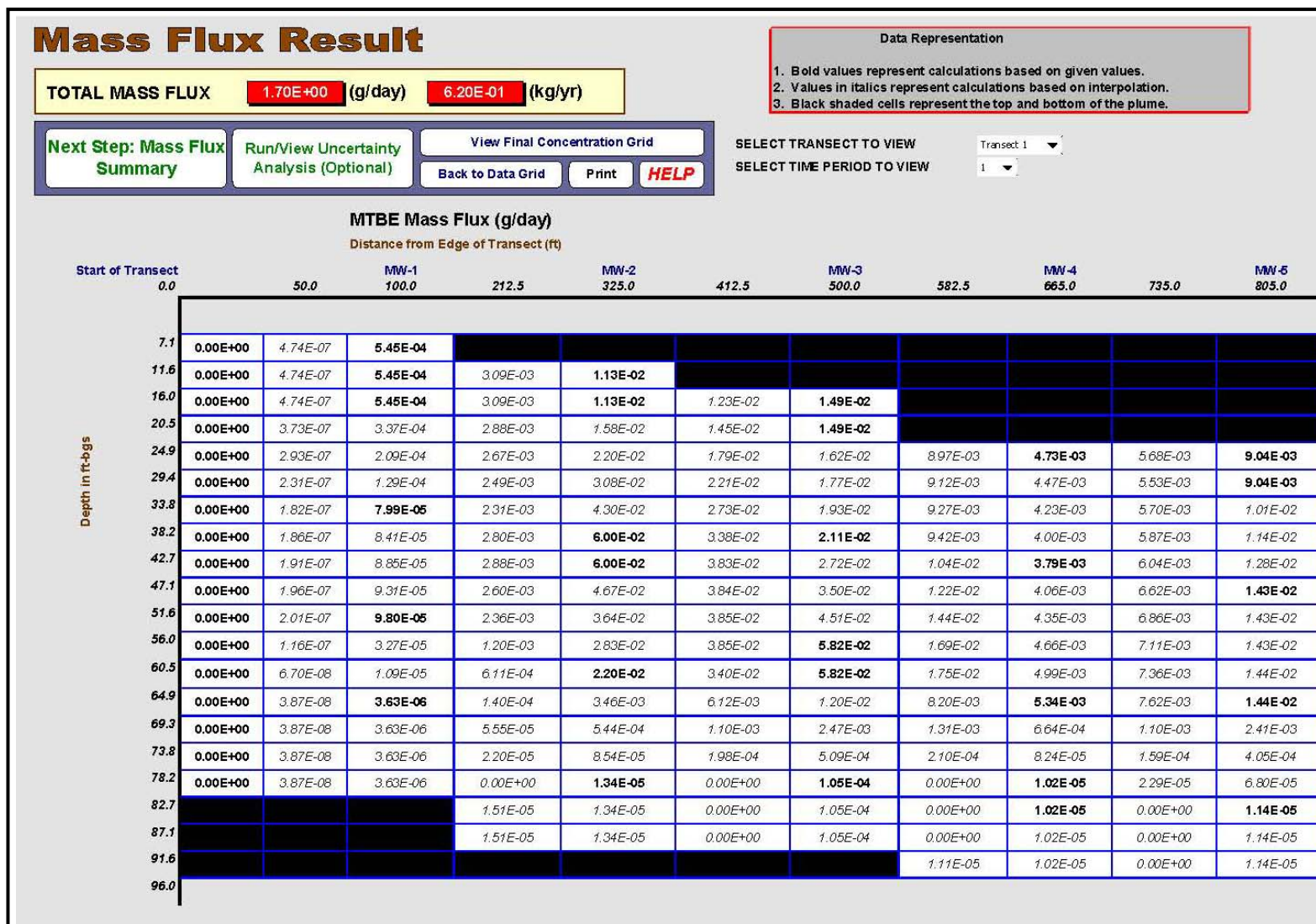


Figure 3-30. MTBE Log Transformation: Mass Flux Results Grid – Page 1

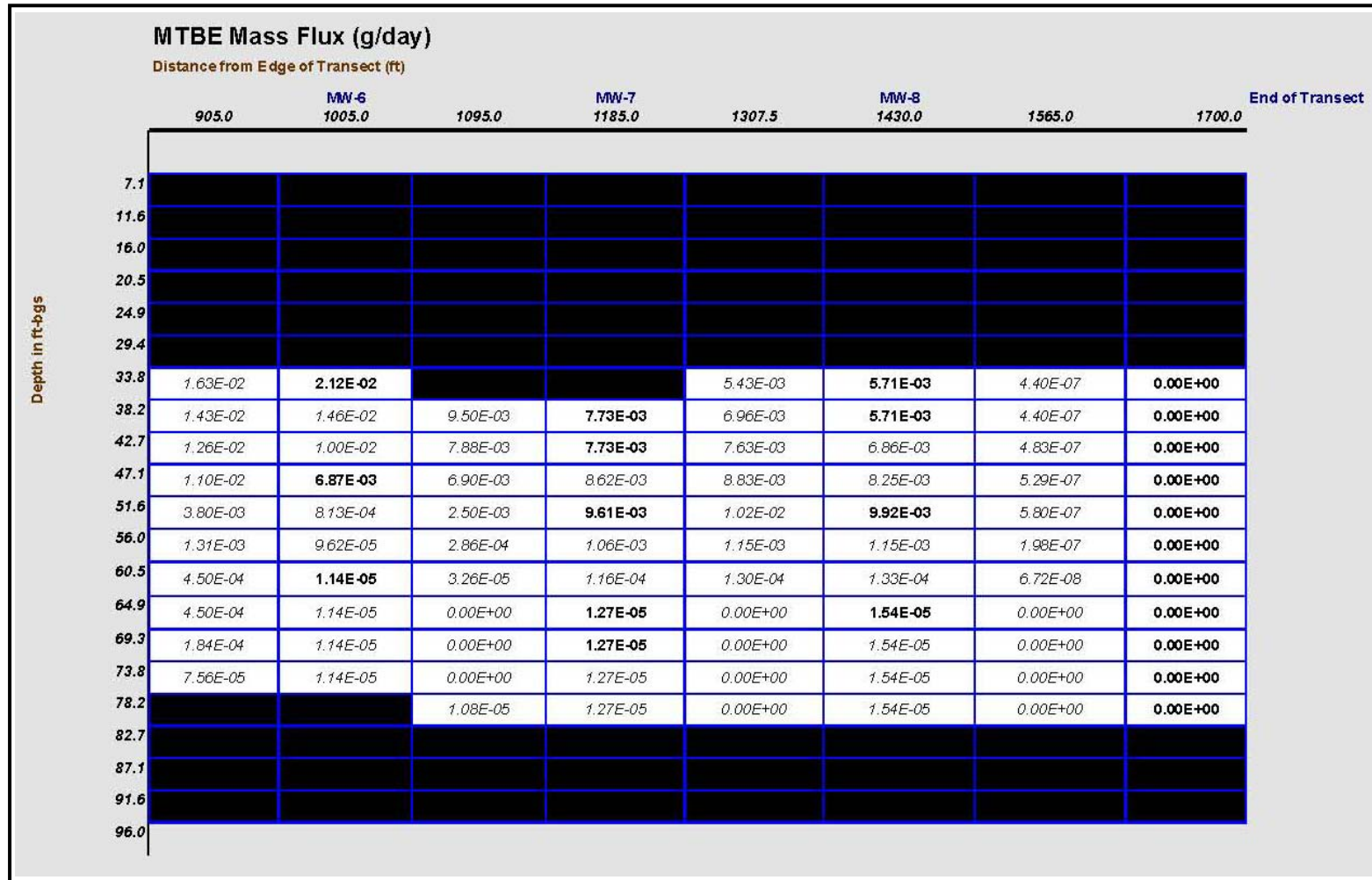


Figure 3-31. MTBE Log Transformation: Mass Flux Results Grid – Page 2

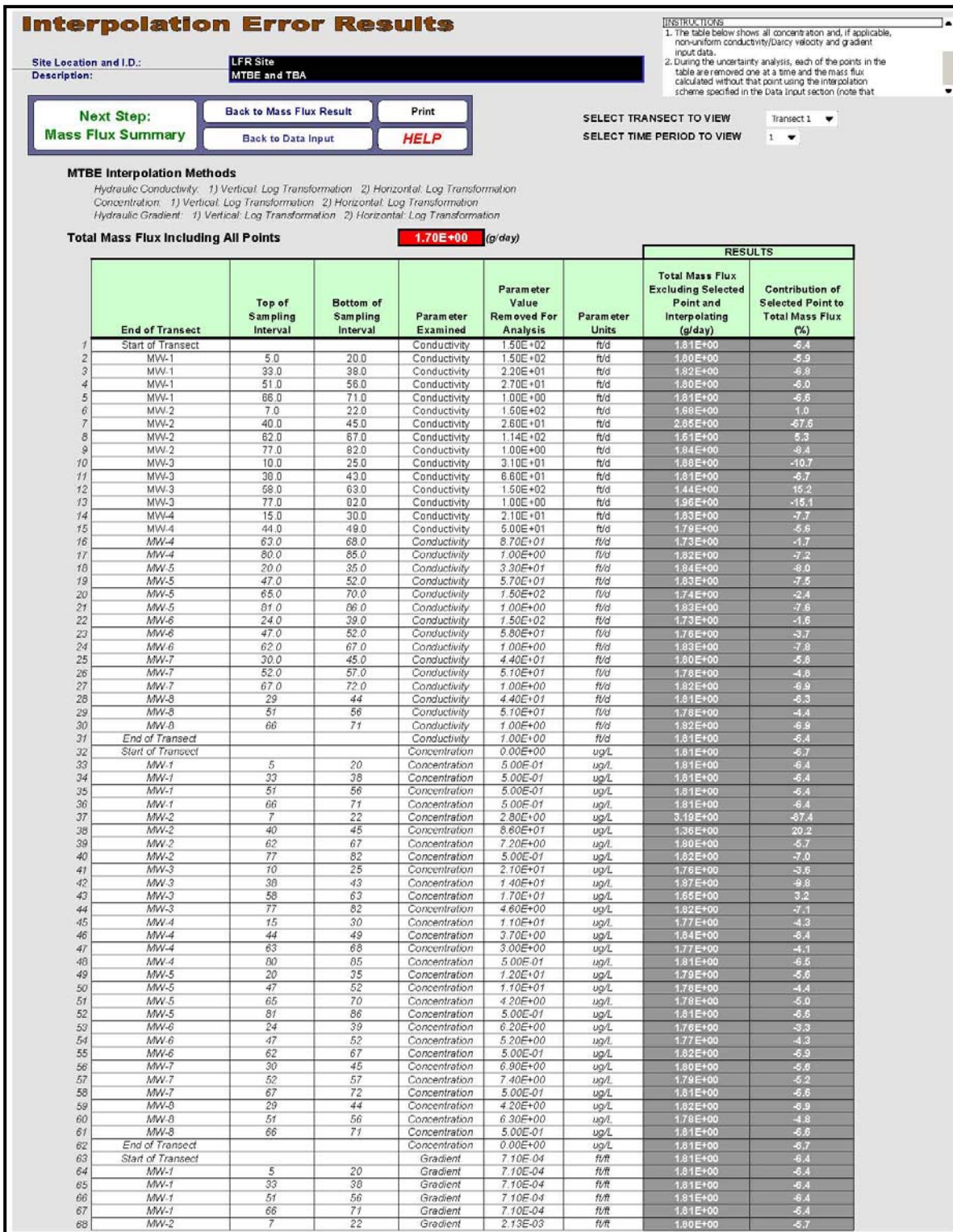


Figure 3-32. MTBE Log Transformation: Simple Uncertainty Analysis – Page 1

CASE STUDY: MTBE AND TBA

							RESULTS	
	End of Transect	Top of Sampling Interval	Bottom of Sampling Interval	Parameter Examined	Parameter Value Removed For Analysis	Parameter Units	Total Mass Flux Excluding Selected Point and Interpolating (g/day)	Contribution of Selected Point to Total Mass Flux (%)
69	MW-2	40	45	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
70	MW-2	62	67	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
71	MW-2	77	82	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
72	MW-3	10	25	Gradient	2.13E-03	ft/ft	1.79E+00	-5.5
73	MW-3	38	43	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
74	MW-3	58	63	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
75	MW-3	77	82	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
76	MW-4	15	30	Gradient	2.13E-03	ft/ft	1.80E+00	-5.8
77	MW-4	44	49	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
78	MW-4	63	68	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
79	MW-4	80	85	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
80	MW-5	20	35	Gradient	2.13E-03	ft/ft	1.80E+00	-5.8
81	MW-5	47	52	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
82	MW-5	65	70	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
83	MW-5	81	86	Gradient	2.13E-03	ft/ft	1.81E+00	-6.4
84	MW-6	24	39	Gradient	1.91E-03	ft/ft	1.77E+00	-3.9
85	MW-6	47	52	Gradient	1.91E-03	ft/ft	1.81E+00	-6.4
86	MW-6	62	67	Gradient	1.91E-03	ft/ft	1.81E+00	-6.4
87	MW-7	30	45	Gradient	1.91E-03	ft/ft	1.79E+00	-5.5
88	MW-7	52	57	Gradient	1.91E-03	ft/ft	1.81E+00	-6.4
89	MW-7	67	72	Gradient	1.91E-03	ft/ft	1.81E+00	-6.4
90	MW-8	29	44	Gradient	1.91E-03	ft/ft	1.80E+00	-6.0
91	MW-8	51	56	Gradient	1.91E-03	ft/ft	1.81E+00	-6.4
92	MW-8	66	71	Gradient	1.91E-03	ft/ft	1.81E+00	-6.4
93	End of Transect			Gradient	1.91E-03	ft/ft	1.81E+00	-6.4

Figure 3-33. MTBE Log Transformation: Simple Uncertainty Analysis – Page 2

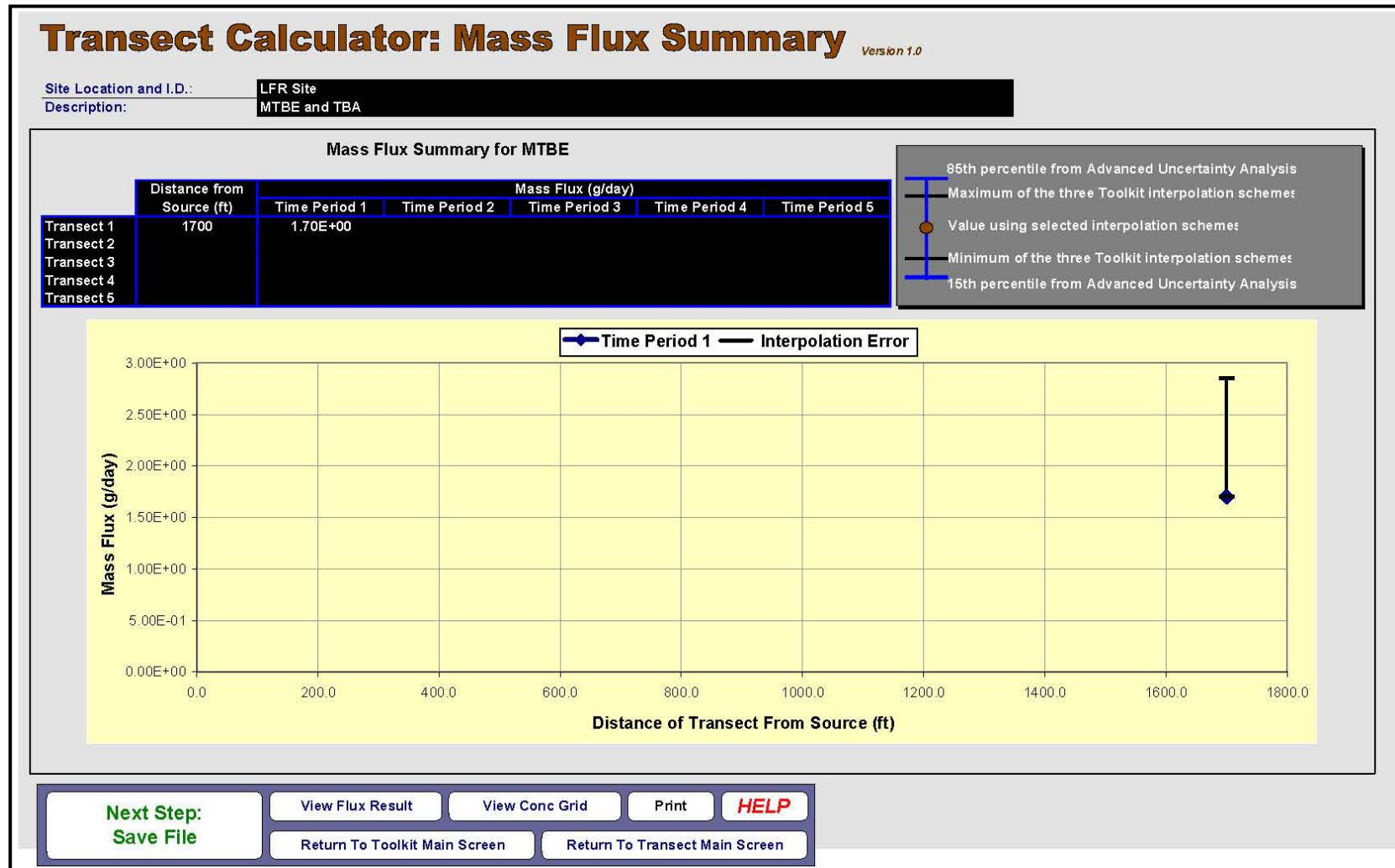


Figure 3-34. MTBE Log Transformation: Mass Flux Summary

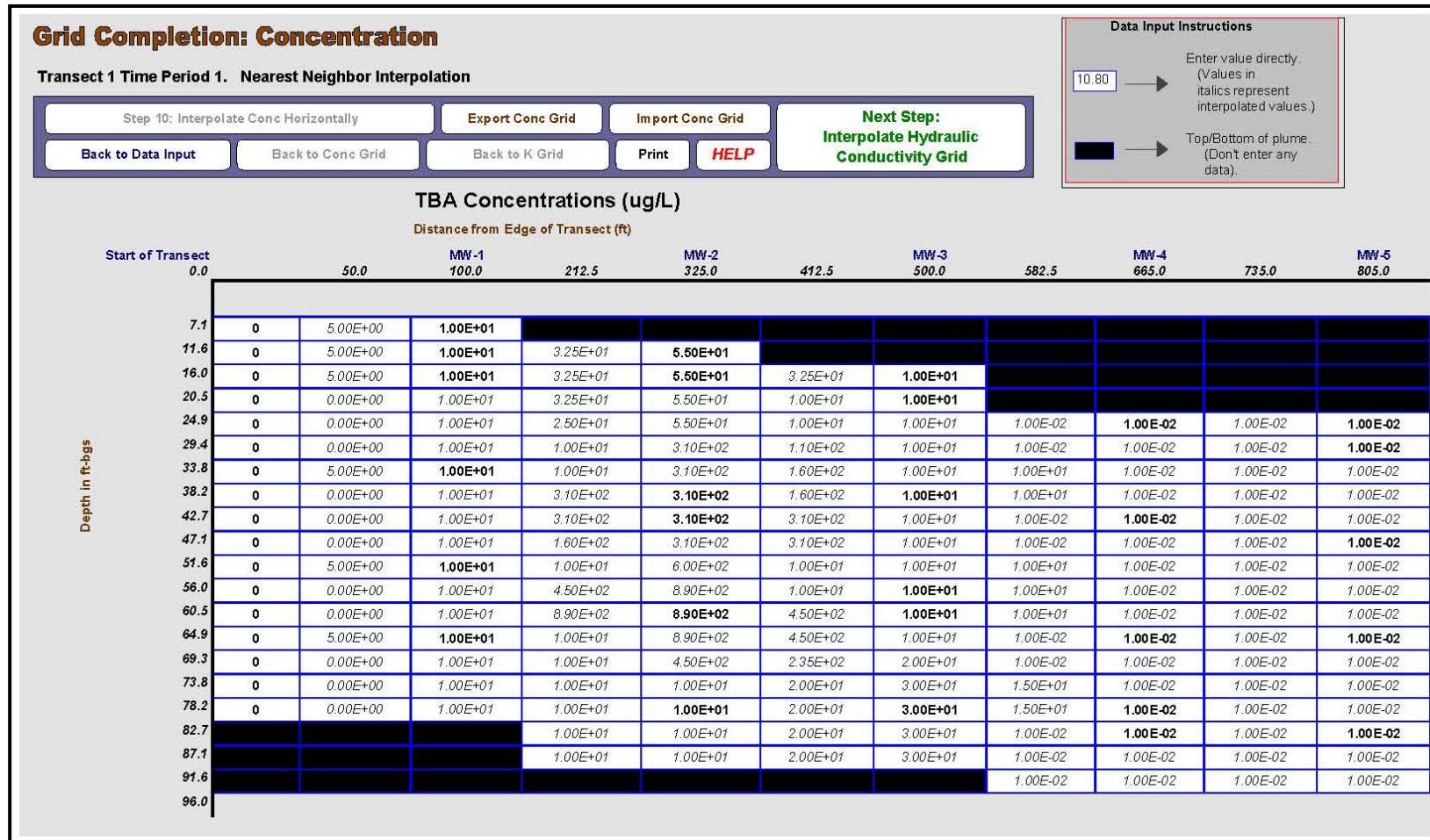


Figure 3-35. TBA Nearest Neighbor Interpolation: Concentration Grid – Page 1

CASE STUDY: MTBE AND TBA

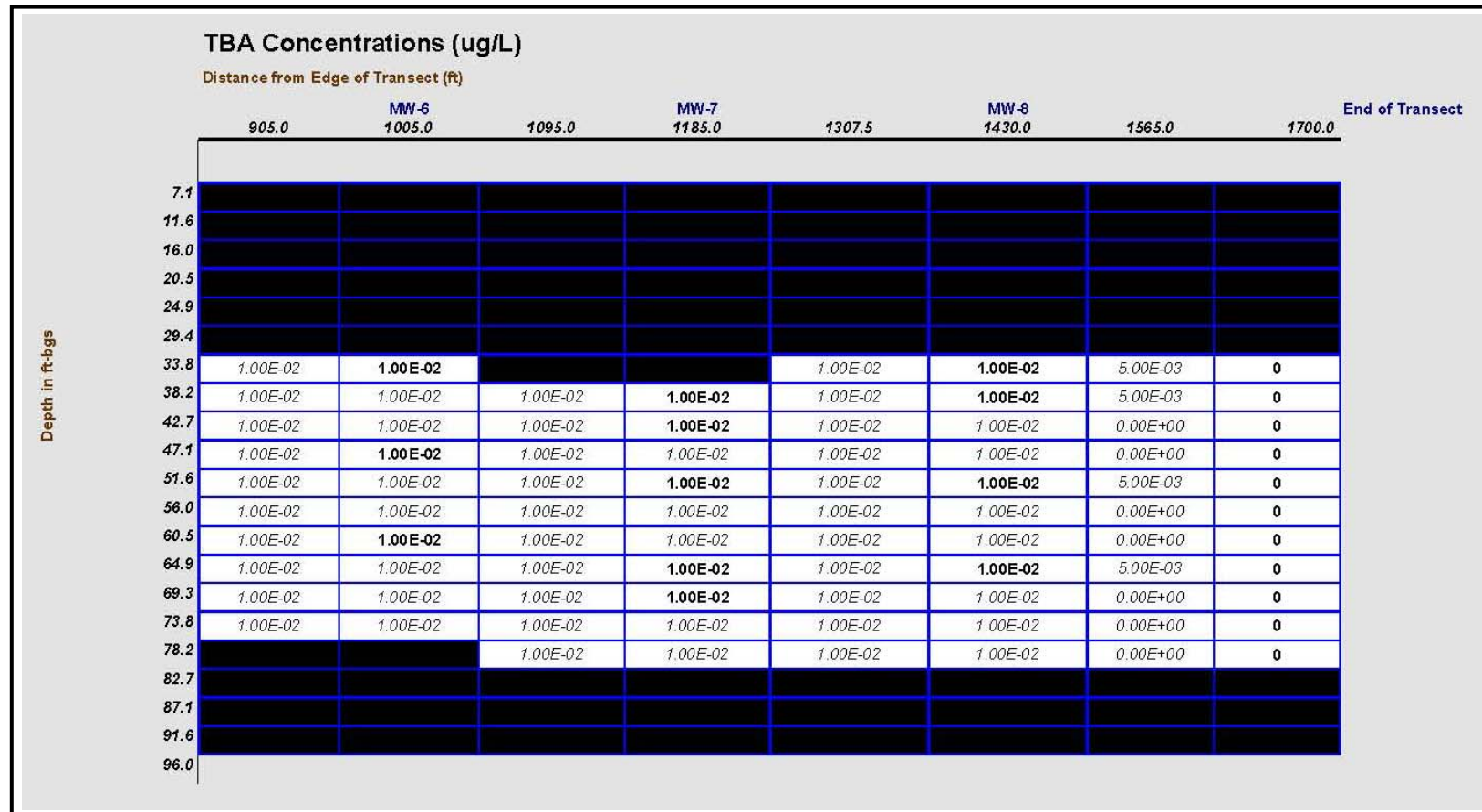


Figure 3-36. TBA Nearest Neighbor Interpolation: Concentration Grid – Page 2

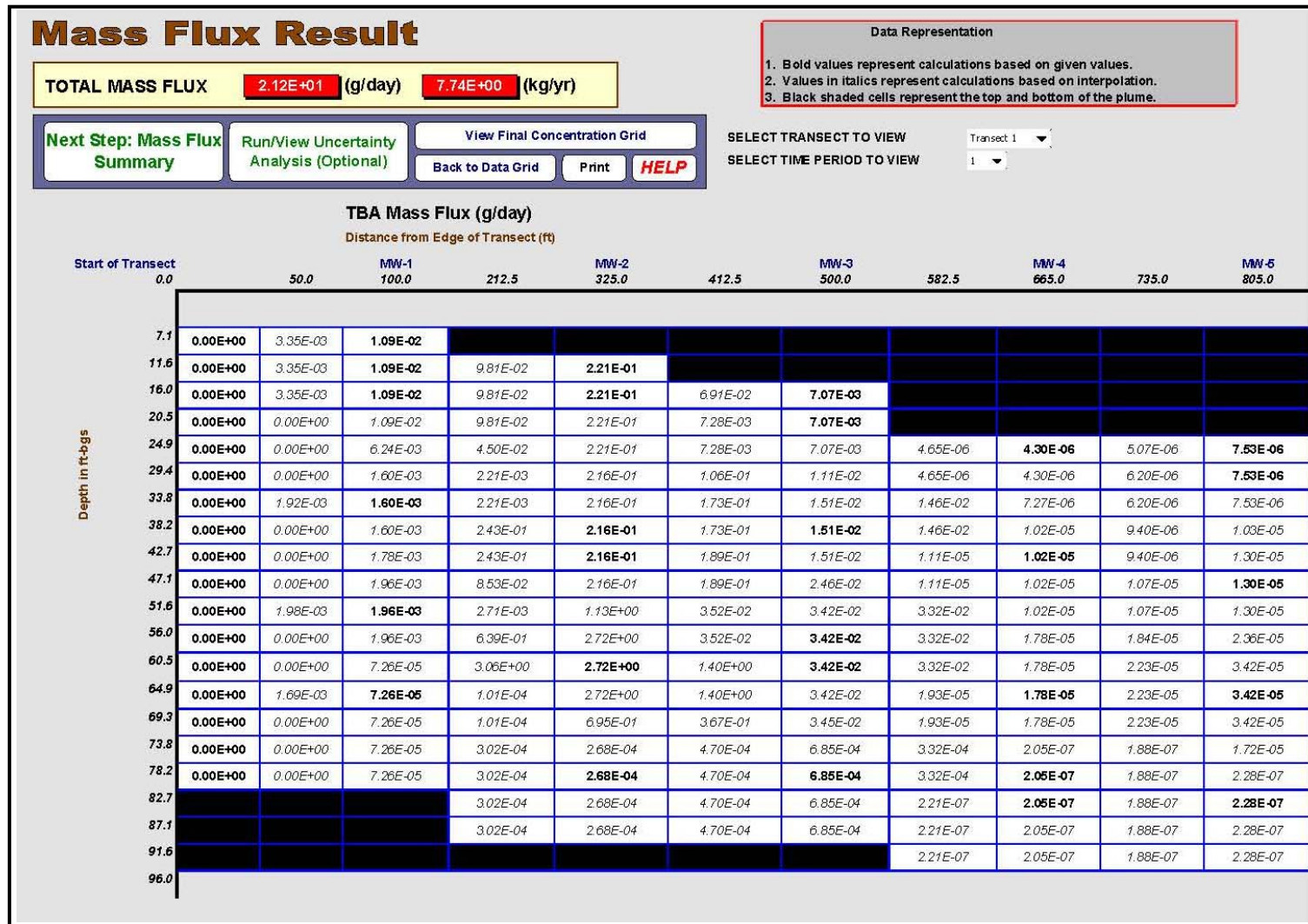


Figure 3-37. TBA Nearest Neighbor Interpolation: Mass Flux Results Grid – Page 1
 (For conductivity and gradient grids see Figures 3-6 through 3-9)

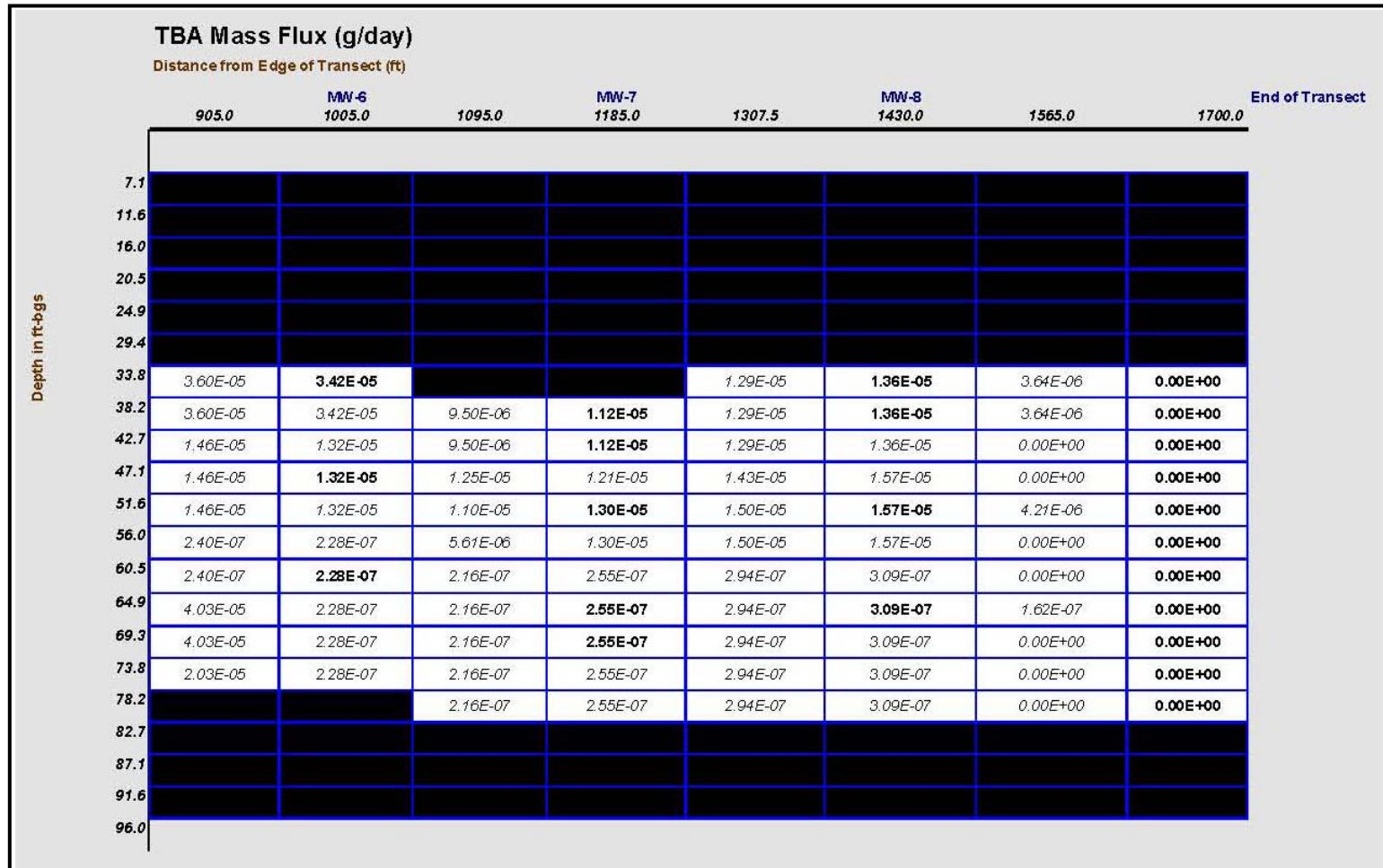


Figure 3-38. TBA Nearest Neighbor Interpolation: Mass Flux Results Grid – Page 2
(For conductivity and gradient grids see Figures 3-6 through 3-9)

CASE STUDY: MTBE AND TBA

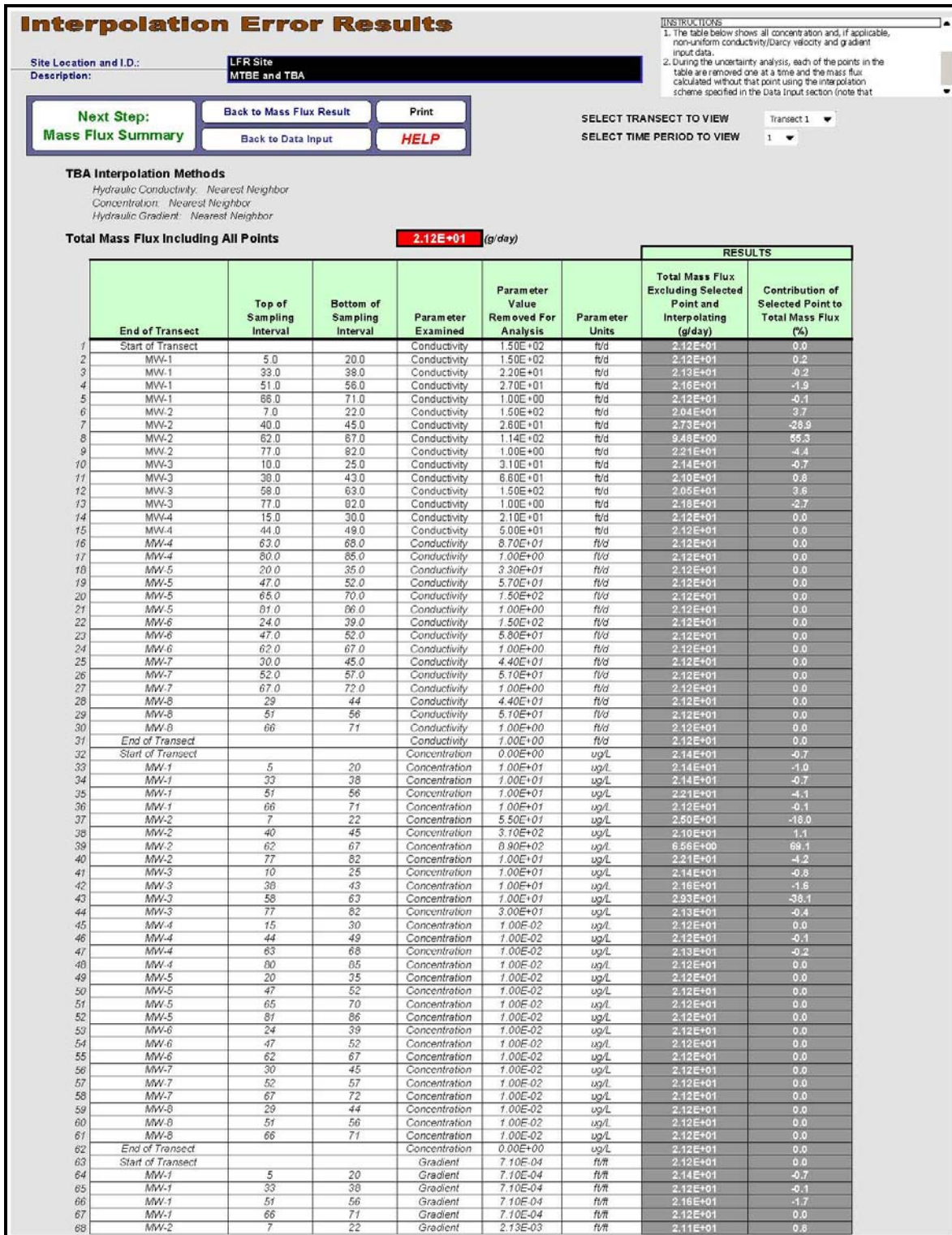


Figure 3-39. TBA Nearest Neighbor Interpolation: Simple Uncertainty Analysis – Page 1

CASE STUDY: MTBE AND TBA

							RESULTS	
	End of Transect	Top of Sampling Interval	Bottom of Sampling Interval	Parameter Examined	Parameter Value Removed For Analysis	Parameter Units	Total Mass Flux Excluding Selected Point and Interpolating (g/day)	Contribution of Selected Point to Total Mass Flux (%)
69	MW-2	40	45	Gradient	2.13E-03	ft/ft	2.08E+01	1.7
70	MW-2	62	67	Gradient	2.13E-03	ft/ft	1.89E+01	11.1
71	MW-2	77	82	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
72	MW-3	10	25	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
73	MW-3	38	43	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
74	MW-3	58	63	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
75	MW-3	77	82	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
76	MW-4	15	30	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
77	MW-4	44	49	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
78	MW-4	63	68	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
79	MW-4	80	85	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
80	MW-5	20	35	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
81	MW-5	47	52	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
82	MW-5	65	70	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
83	MW-5	81	86	Gradient	2.13E-03	ft/ft	2.12E+01	0.0
84	MW-6	24	39	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
85	MW-6	47	52	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
86	MW-6	62	67	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
87	MW-7	30	45	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
88	MW-7	52	57	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
89	MW-7	67	72	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
90	MW-8	29	44	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
91	MW-8	51	56	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
92	MW-8	66	71	Gradient	1.91E-03	ft/ft	2.12E+01	0.0
93	End of Transect			Gradient	1.91E-03	ft/ft	2.12E+01	0.0

Figure 3-40. TBA Nearest Neighbor Interpolation: Simple Uncertainty Analysis – Page 2

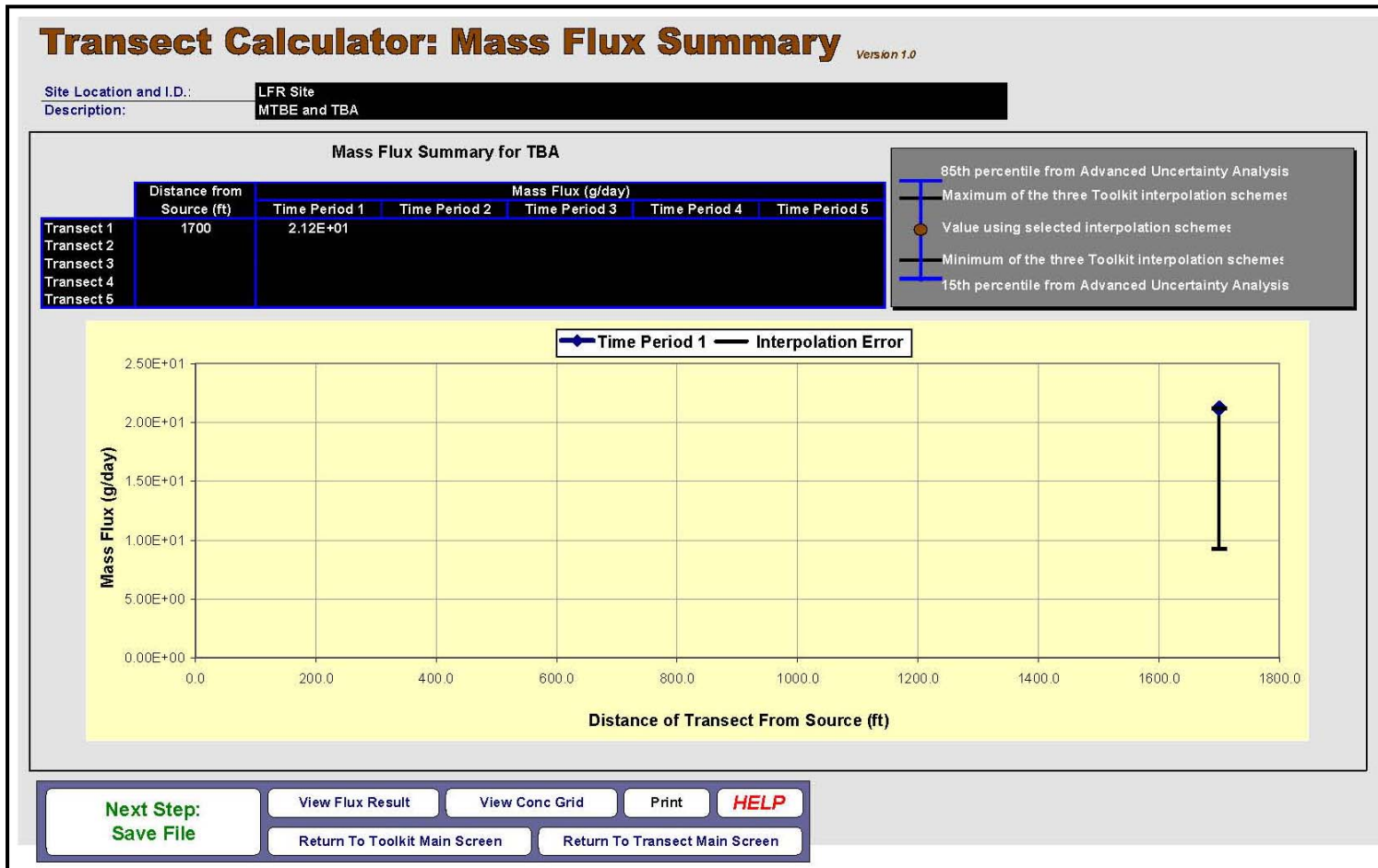


Figure 3-41. TBA Nearest Neighbor Interpolation: Mass Flux Summary

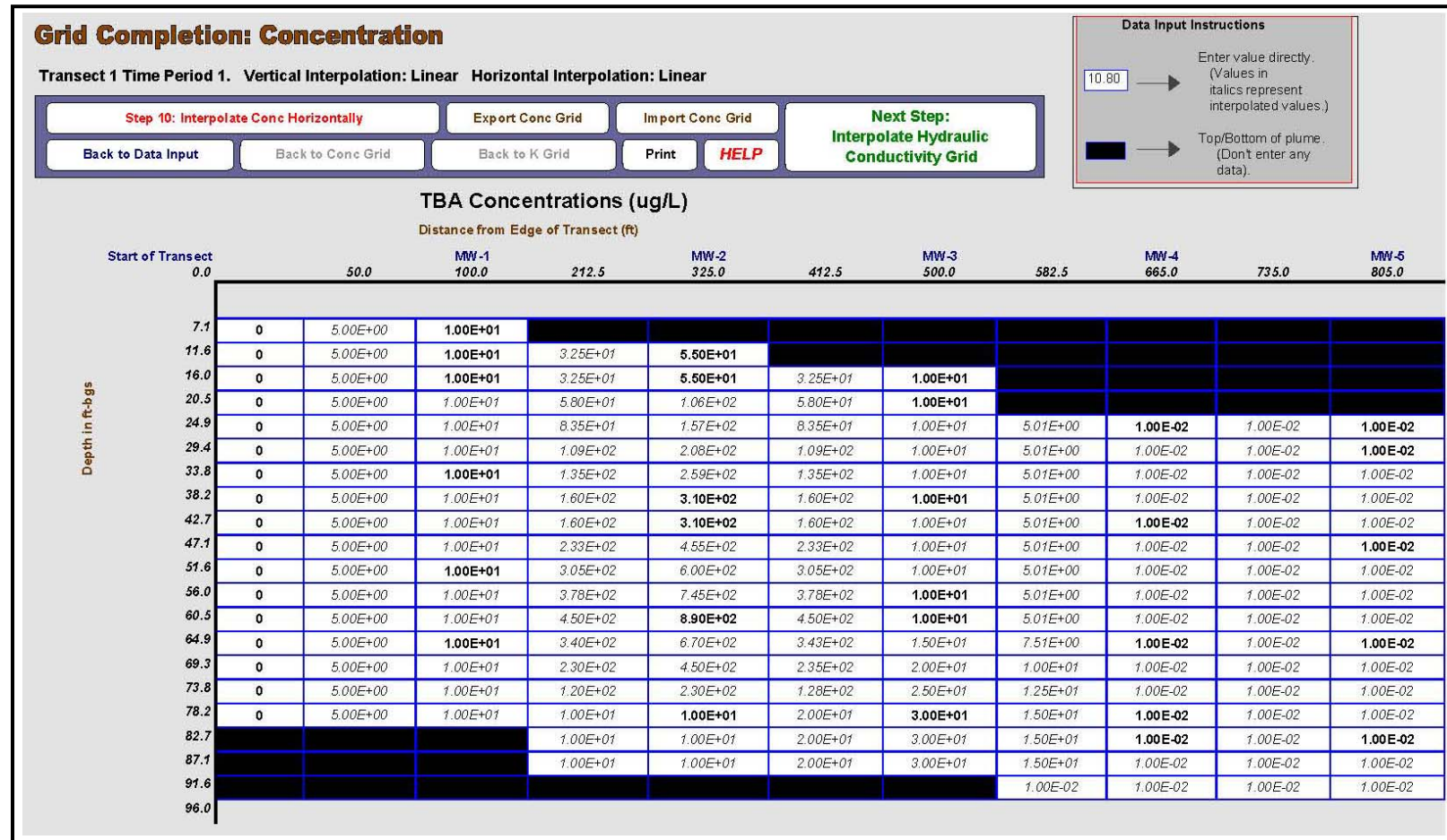


Figure 3-42. TBA Linear Interpolation: Concentration Grid – Page 1

CASE STUDY: MTBE AND TBA

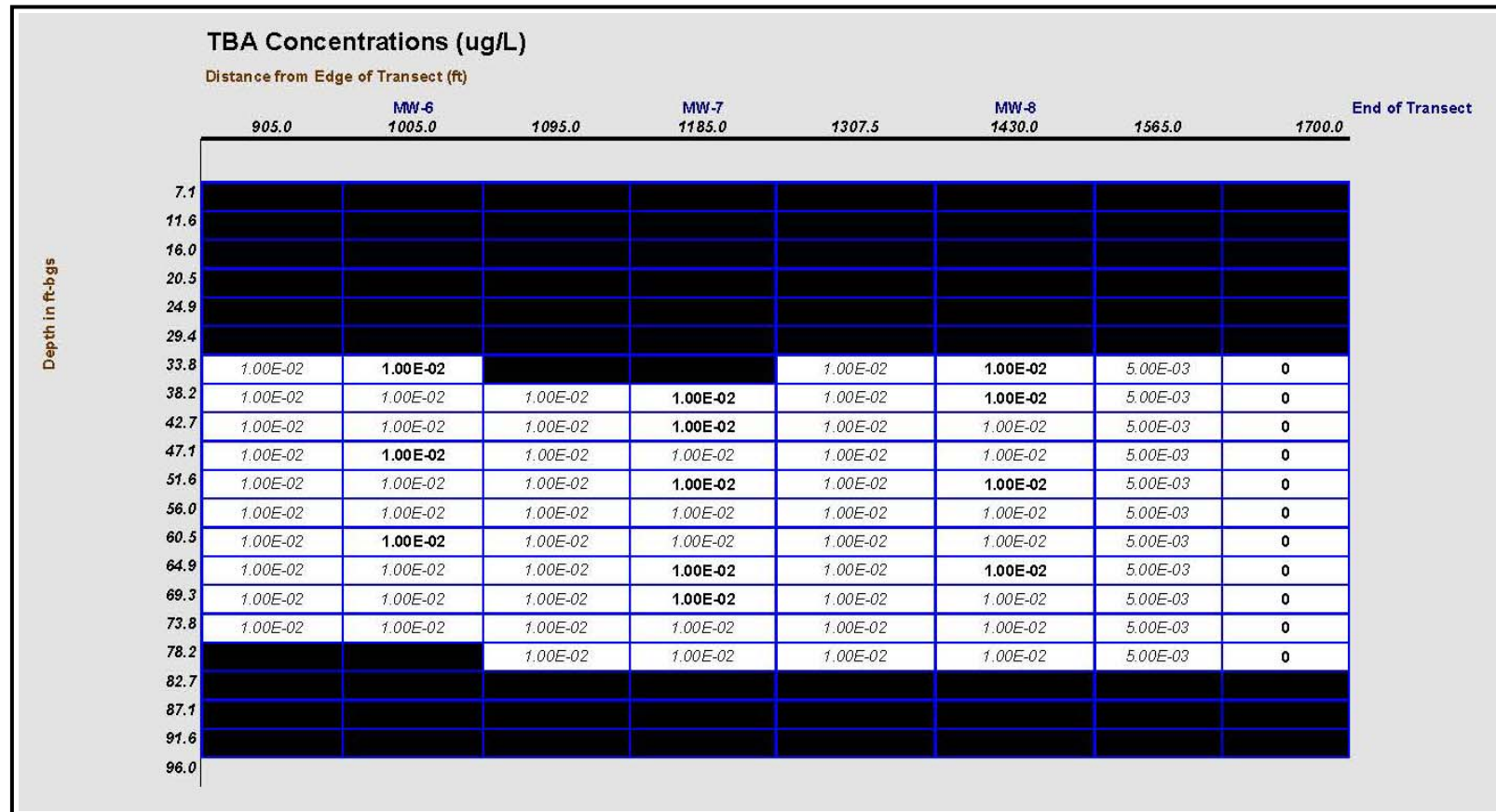


Figure 3-43. TBA Linear Interpolation: Concentration Grid – Page 2

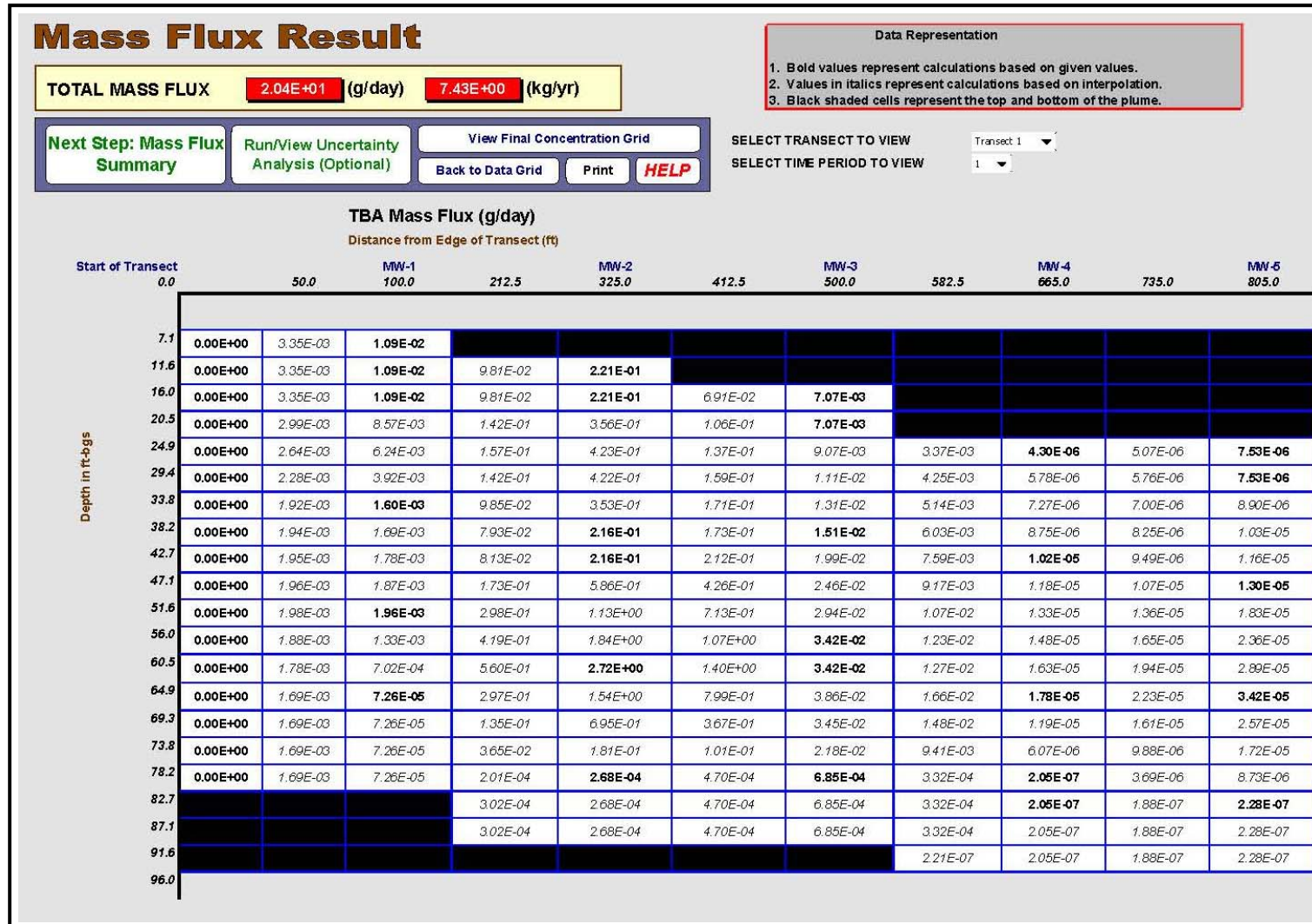


Figure 3-44. TBA Linear Interpolation: Mass Flux Results Grid – Page 1
 (For conductivity and gradient grids see Figures 3-15 through 3-18)

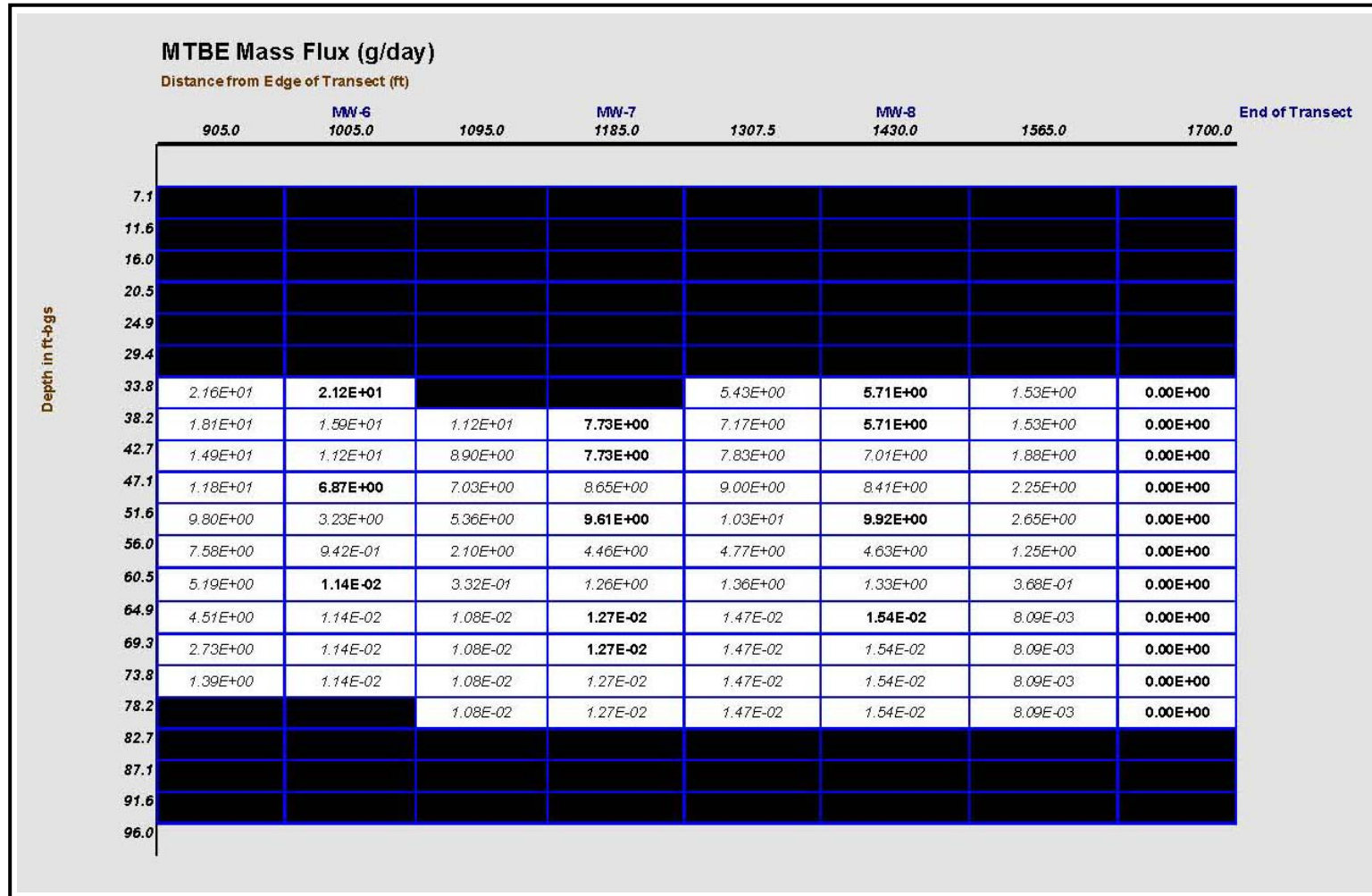


Figure 3-45. TBA Linear Interpolation: Mass Flux Results Grid – Page 2
(For conductivity and gradient grids see Figures 3-15 through 3-18)

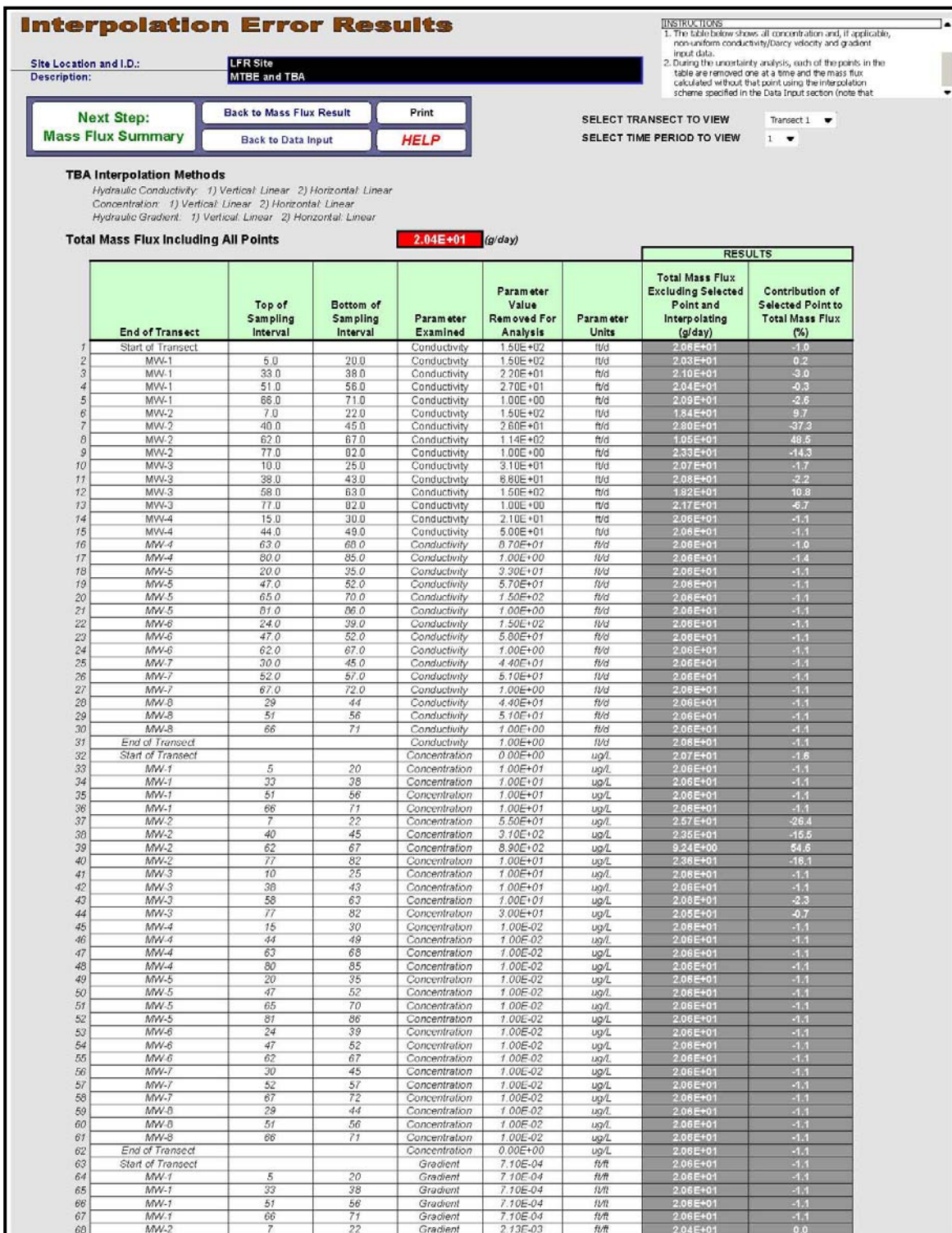


Figure 3-46. TBA Linear Interpolation: Simple Uncertainty Analysis – Page 1

CASE STUDY: MTBE AND TBA

						RESULTS		
	End of Transect	Top of Sampling Interval	Bottom of Sampling Interval	Parameter Examined	Parameter Value Removed For Analysis	Parameter Units	Total Mass Flux Excluding Selected Point and Interpolating (g/day)	Contribution of Selected Point to Total Mass Flux (%)
69	MW-2	40	45	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
70	MW-2	62	67	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
71	MW-2	77	82	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
72	MW-3	10	25	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
73	MW-3	38	43	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
74	MW-3	58	63	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
75	MW-3	77	82	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
76	MW-4	15	30	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
77	MW-4	44	49	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
78	MW-4	63	68	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
79	MW-4	80	85	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
80	MW-5	20	35	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
81	MW-5	47	52	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
82	MW-5	65	70	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
83	MW-5	81	86	Gradient	2.13E-03	ft/ft	2.06E+01	-1.1
84	MW-6	24	39	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
85	MW-6	47	52	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
86	MW-6	62	67	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
87	MW-7	30	45	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
88	MW-7	52	57	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
89	MW-7	67	72	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
90	MW-8	29	44	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
91	MW-8	51	56	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
92	MW-8	66	71	Gradient	1.91E-03	ft/ft	2.06E+01	-1.1
93	End of Transect			Gradient	1.91E-03	ft/ft	2.06E+01	-1.1

Figure 3-47. TBA Linear Interpolation: Simple Uncertainty Analysis – Page 2

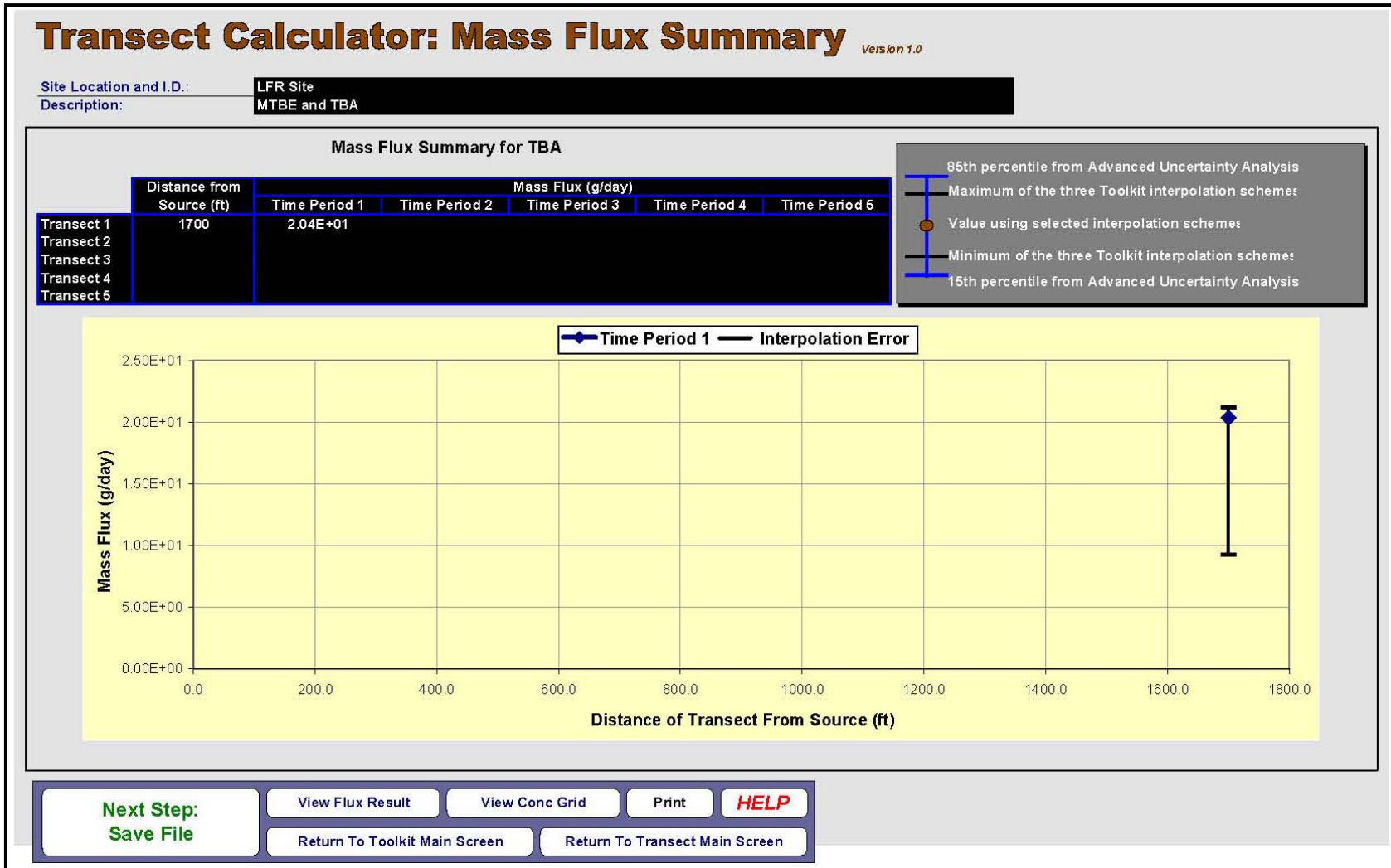


Figure 3-48. TBA Linear Interpolation: Mass Flux Summary

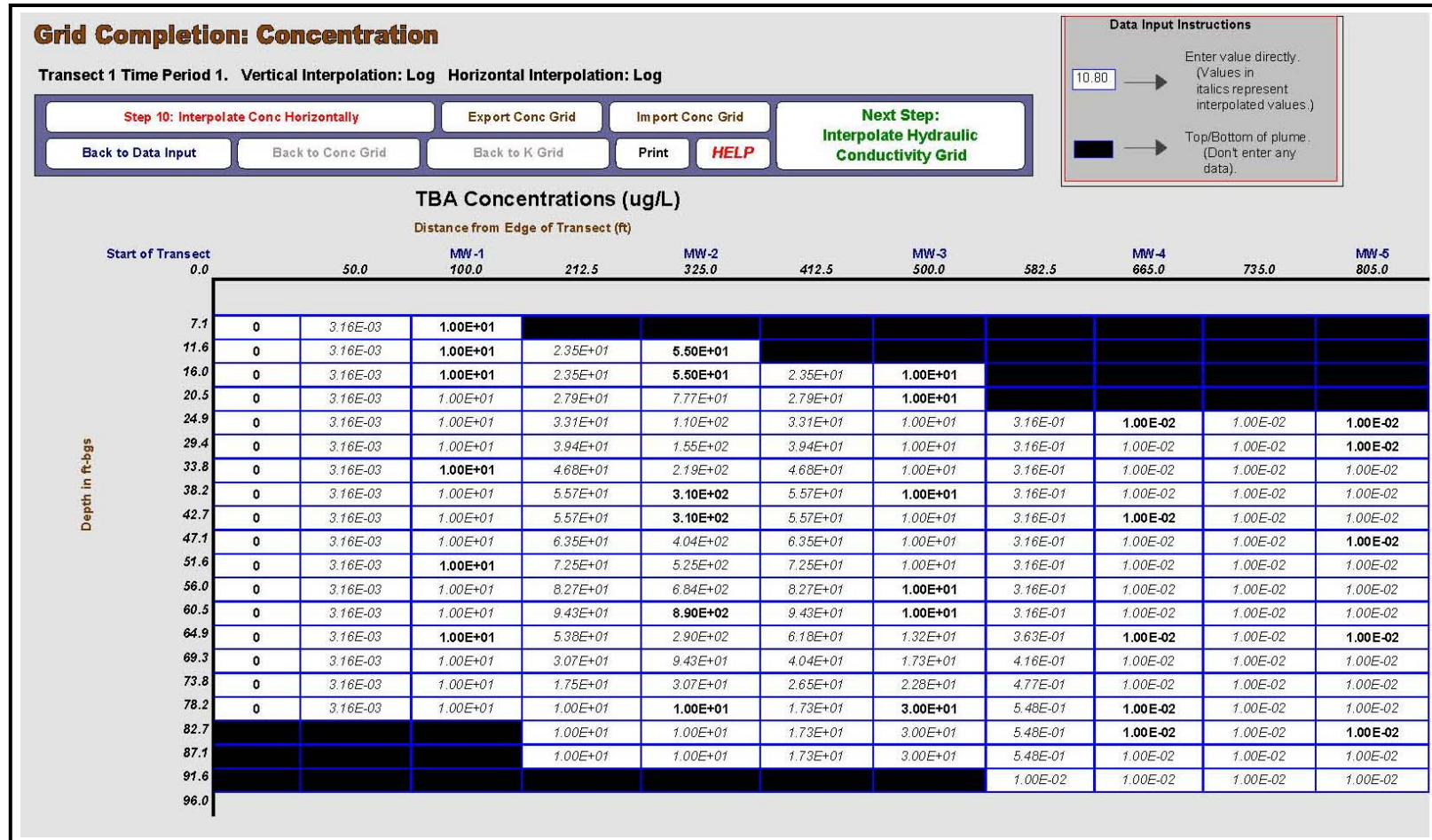


Figure 3-49. TBA Log Transformation: Concentration Grid – Page 1

CASE STUDY: MTBE AND TBA

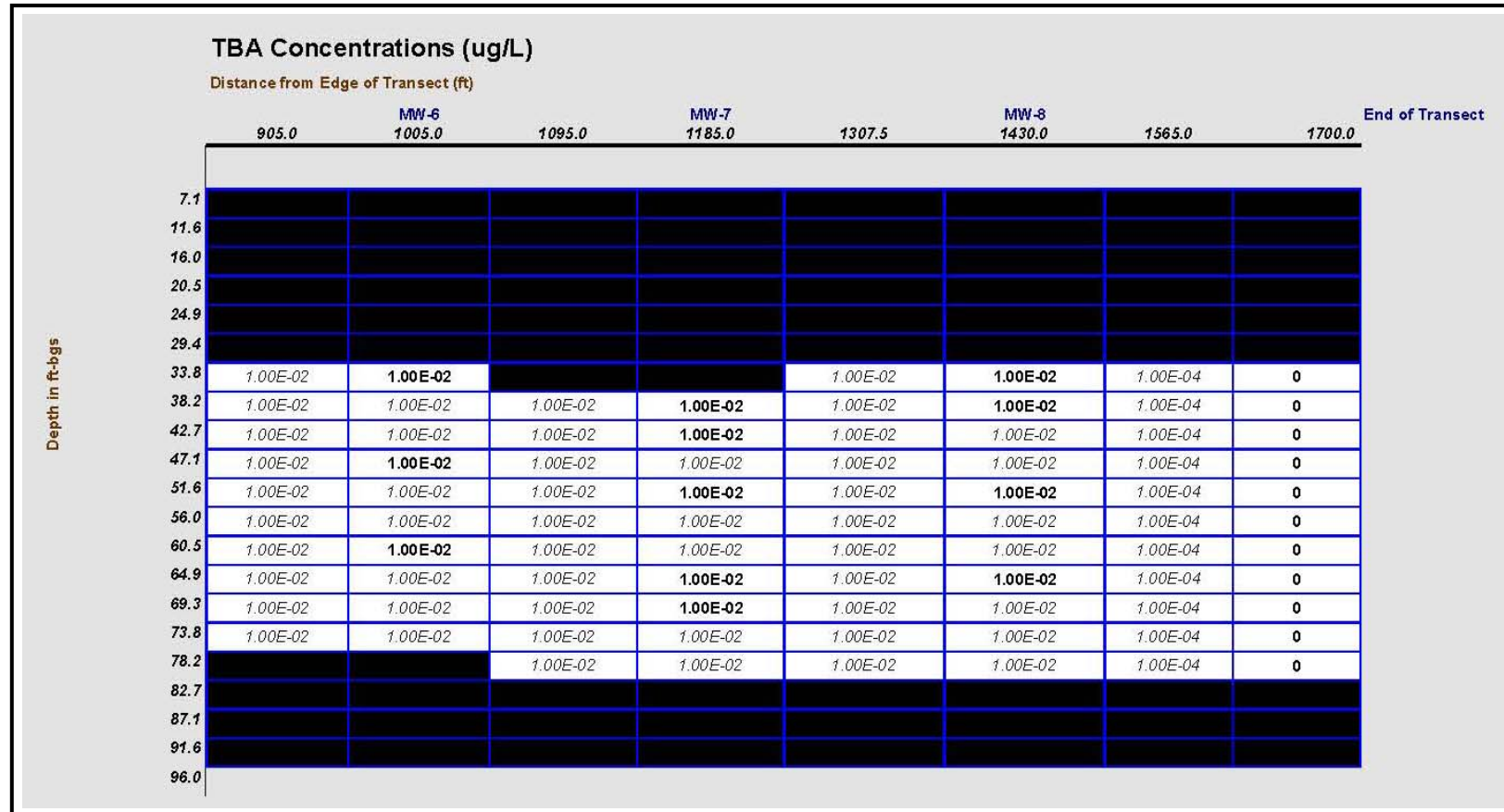


Figure 3-50. TBA Log Transformation: Concentration Grid – Page 2

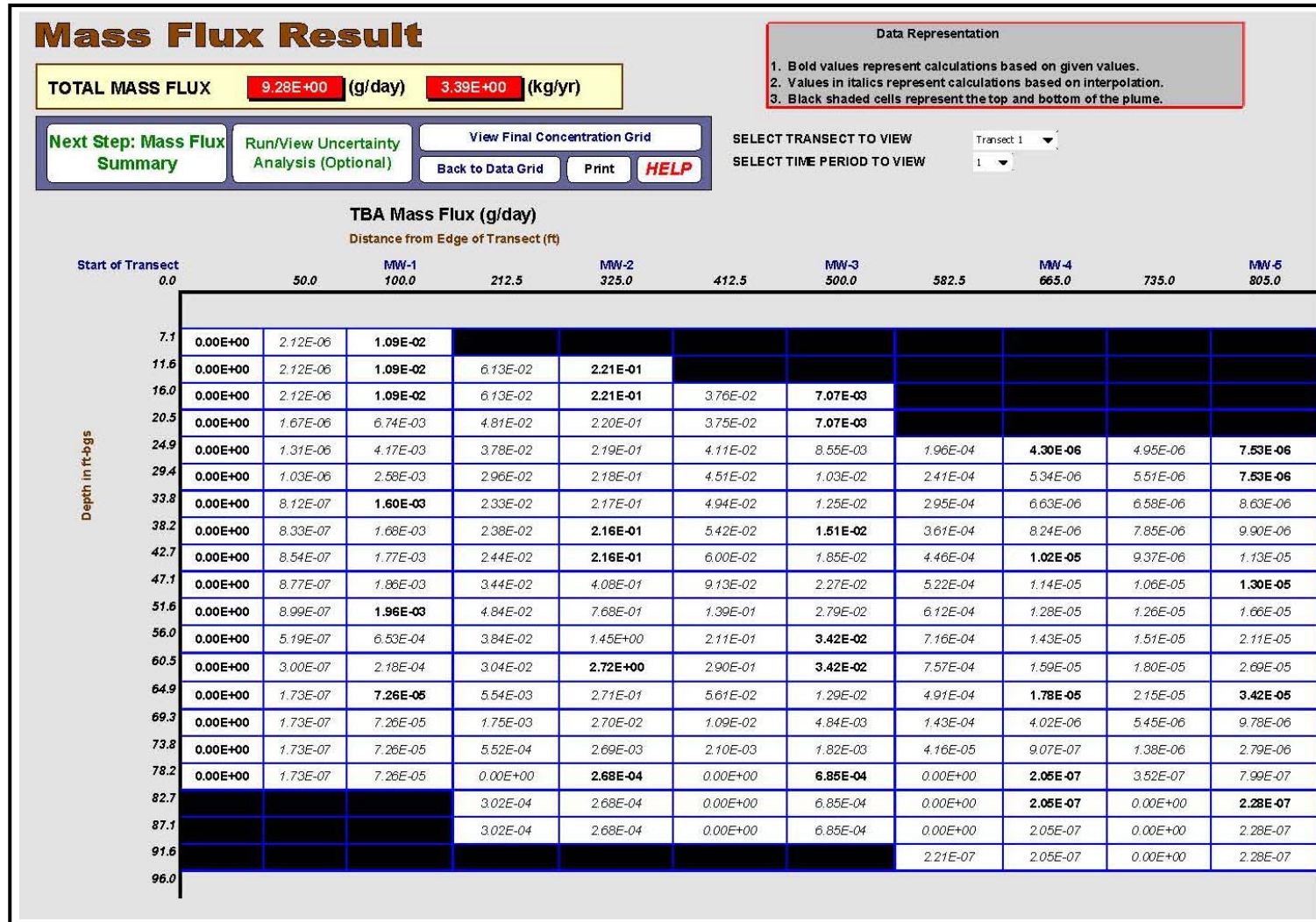


Figure 3-51. TBA Log Transformation: Mass Flux Results Grid – Page 1
(For conductivity and gradient grids see Figures 3-26 through 3-29)

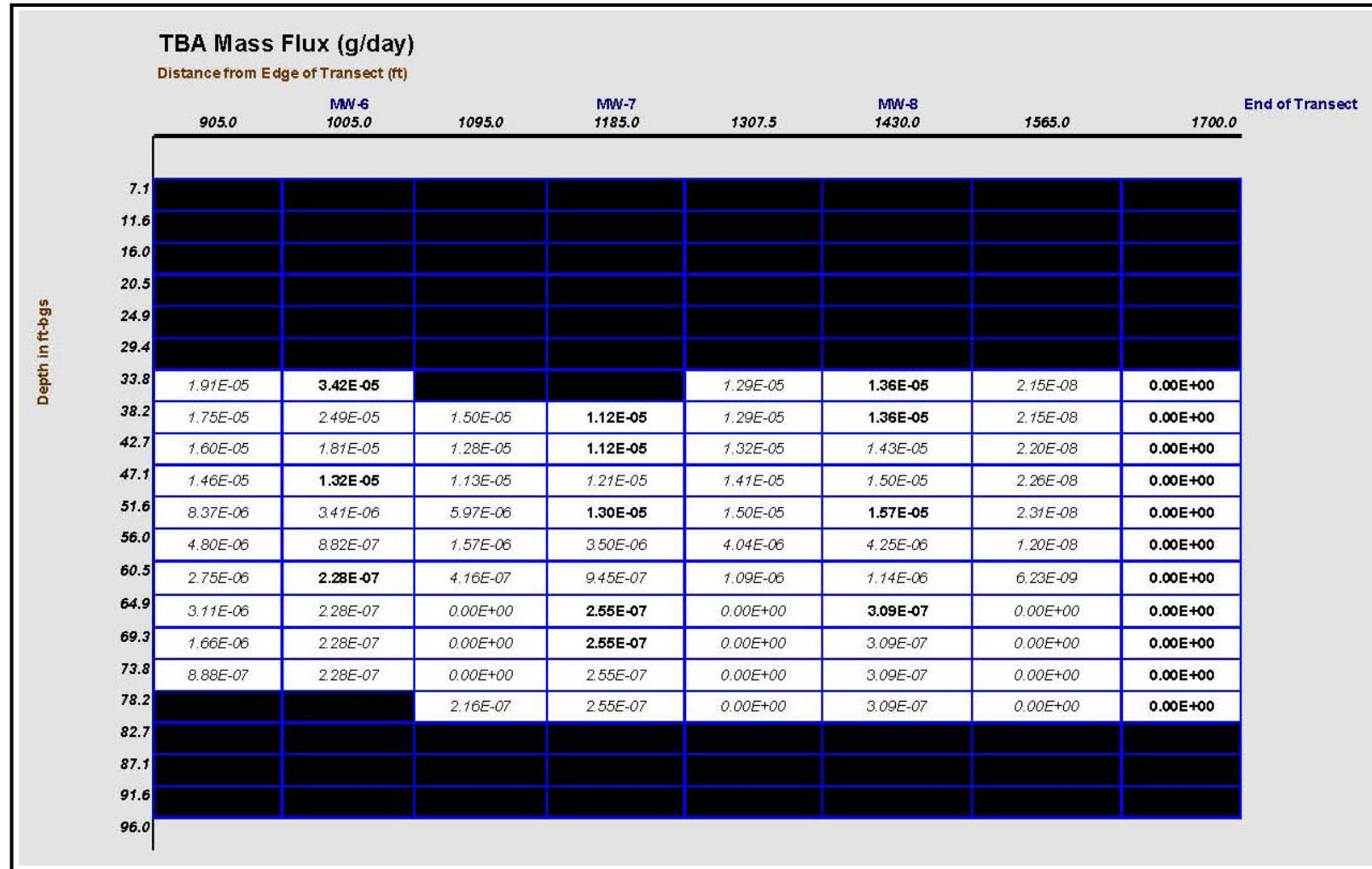


Figure 3-52. TBA Log Transformation: Mass Flux Results Grid – Page 2
(For conductivity and gradient grids see Figures 3-26 through 3-29)

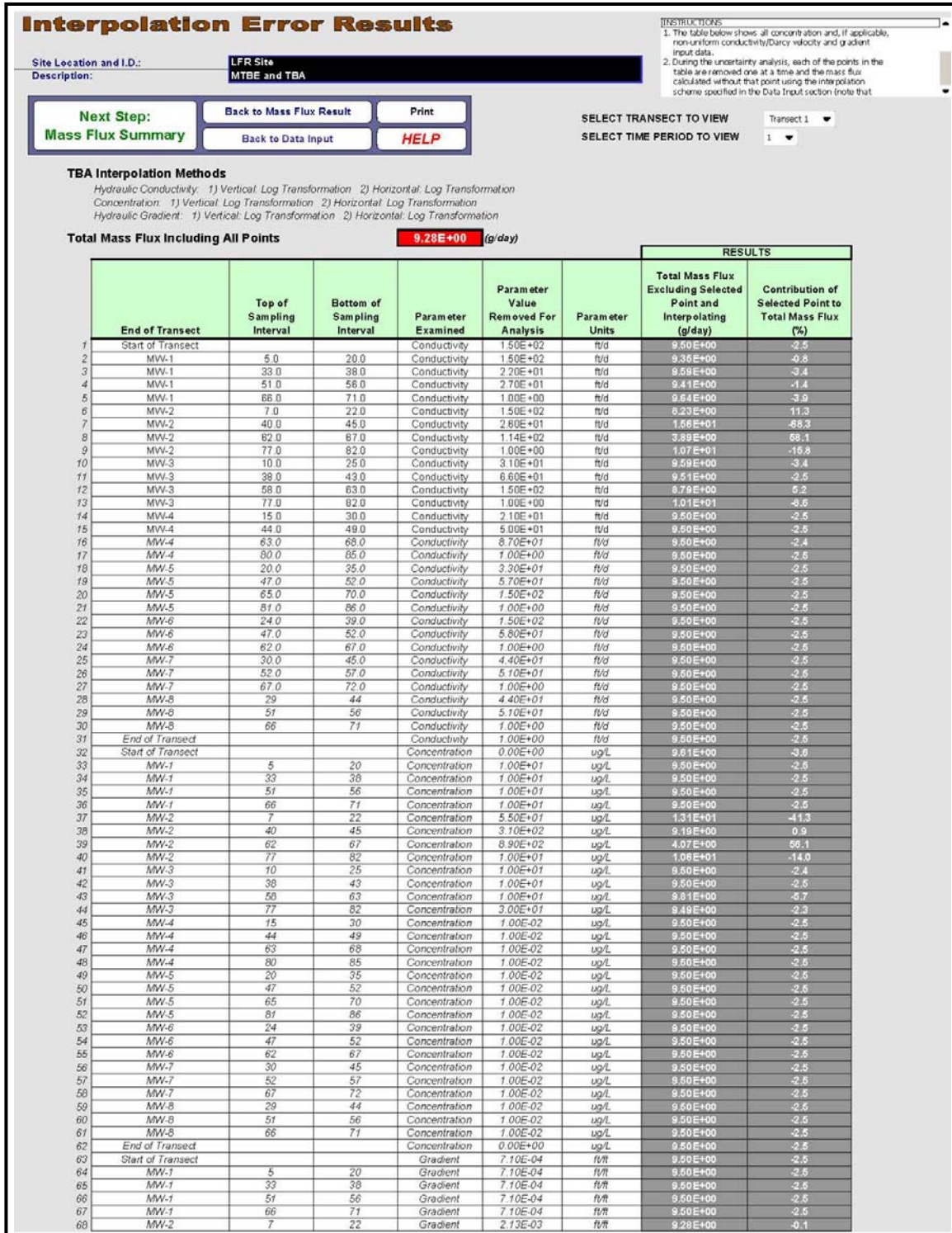


Figure 3-53. TBA Log Transformation: Simple Uncertainty Analysis – Page 1

CASE STUDY: MTBE AND TBA

							RESULTS	
	End of Transect	Top of Sampling Interval	Bottom of Sampling Interval	Parameter Examined	Parameter Value Removed For Analysis	Parameter Units	Total Mass Flux Excluding Selected Point and Interpolating (g/day)	Contribution of Selected Point to Total Mass Flux (%)
69	MW-2	40	45	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
70	MW-2	62	67	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
71	MW-2	77	82	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
72	MW-3	10	25	Gradient	2.13E-03	ft/ft	9.50E+00	-2.4
73	MW-3	38	43	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
74	MW-3	58	63	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
75	MW-3	77	82	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
76	MW-4	15	30	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
77	MW-4	44	49	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
78	MW-4	63	68	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
79	MW-4	80	85	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
80	MW-5	20	35	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
81	MW-5	47	52	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
82	MW-5	65	70	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
83	MW-5	81	86	Gradient	2.13E-03	ft/ft	9.50E+00	-2.5
84	MW-6	24	39	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
85	MW-6	47	52	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
86	MW-6	62	67	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
87	MW-7	30	45	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
88	MW-7	52	57	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
89	MW-7	67	72	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
90	MW-8	29	44	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
91	MW-8	51	56	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
92	MW-8	66	71	Gradient	1.91E-03	ft/ft	9.50E+00	-2.5
93	End of Transect			Gradient	1.91E-03	ft/ft	9.50E+00	-2.5

Figure 3-54. TBA Log Transformation: Simple Uncertainty Analysis – Page 2

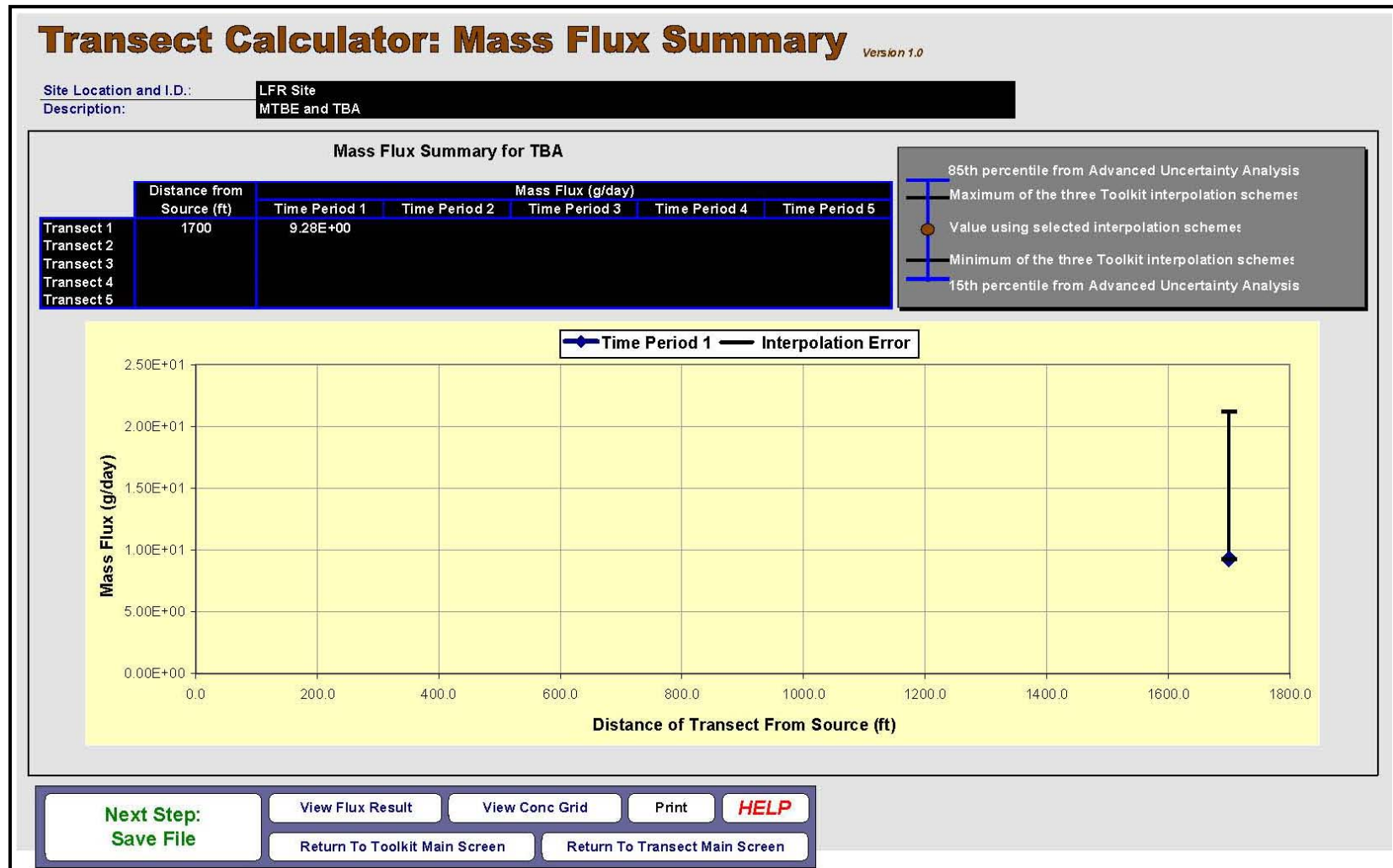


Figure 3-55. TBA Log Transformation: Mass Flux Summary



THIS PAGE LEFT BLANK INTENTIONALLY