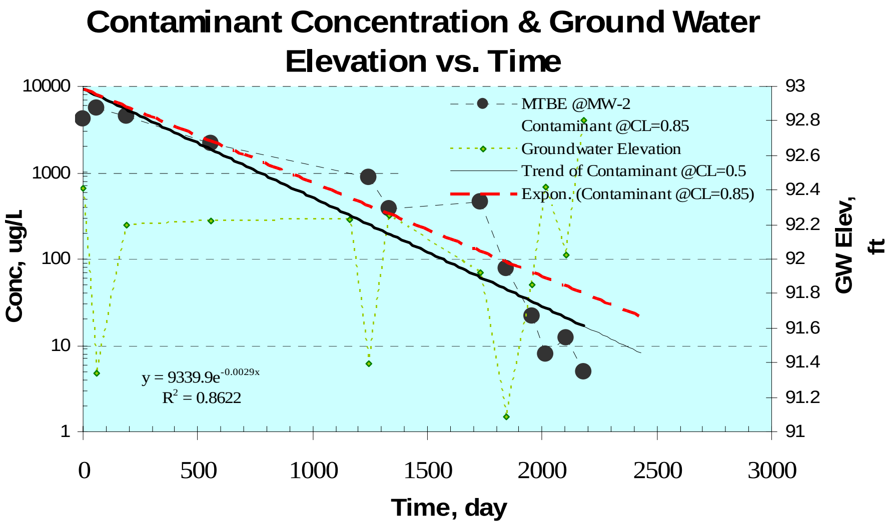
WASHINGTON STATE
DEPARTMENT OF
ECOLOGY

User's Manual:
Natural Attenuation Analysis Tool Package for Petroleum-Contaminated Ground Water

Washington State Department of Ecology
Toxics Cleanup Program

July 2005
Publication No. 05-09-091A *(Version 1.0)*



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This Guidance is available on the Department of Ecology's website at:
http://www.ecy.wa.gov/programs/tcp/policies/pol_main.html

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July 2005

Refer to Publication No. 05-09-091A
Version 1.0

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Hun Seak Park: Washington State Department of Ecology, Toxics Cleanup Program, PO Box 47600, Olympia, WA 98504-7600

Disclaimer: This document is intended to provide guidance under the Model Toxics Control Act (MTCA) Cleanup Regulation, chapter 173-340 WAC, on how to evaluate the feasibility and performance of natural attenuation as a cleanup action for ground water contaminated with petroleum hydrocarbons. It does not establish or modify regulatory requirements. This document is **not** intended, and **cannot** be relied on, to create rights, substantive or procedural, enforceable by any party in litigation with the State of Washington. The Washington State Department of Ecology (Ecology) reserves the right to act at variance with this manual or associated software at any time. Any regulatory decisions made by Ecology in any matter addressed by this guidance will be made by applying the governing statutes and administrative rules to the relevant facts.

The User's Manual, included as part of the natural attenuation guidance package and the associated Data Analysis Tools, available separately, are provided "AS IS" and without warranties as to performance or any other warranties of any kind whether expressed or implied. Although Ecology has provided this User's Manual and associated software Tool Packages to assist in conducting the evaluations, use of these is **not** required to evaluate the feasibility and performance of natural attenuation.

Acknowledgments: The Washington State Department of Ecology thanks Dr. Matthew Small of US EPA Region 9 and Dr. Charles Newell of Groundwater Services, Inc. for critical review and helpful discussions regarding this document.

Contributors (in alphabetical order): **Jerome Cruz, Peter Kmet, and Hun Seak Park**.

With thanks to: Carol Perez, Dan Koroma, Tim Nord, and Jim Pendowski.

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Chapter 1 Introduction

The purpose of this document is to provide detailed technical guidance under the Model Toxics Control Act (MTCA) Cleanup Regulation, chapter 173-340 WAC, on how to evaluate the feasibility and performance of natural attenuation as a cleanup action for ground water contaminated with petroleum hydrocarbons. This document does not provide guidance regarding the establishment of cleanup standards.

This document constitutes one part of the natural attenuation guidance package and consists of the following materials:

- *Guidance on Remediation of Petroleum-Contaminated Ground Water by Natural Attenuation*, Washington State Department of Ecology, Pub. No. 05-09-091 (Guidance)
- ***User's Manual: Natural Attenuation Analysis Tool Package for Petroleum-Contaminated Ground Water,* Washington State Department of Ecology, Pub. No. 05-09-091A (User's Manual) 🡐 THIS DOCUMENT**
- Workbooks: Data Analysis Tool Package: (Two Microsoft Excel® Spreadsheets)

The guidance document (Ecology Pub. No. 05-09-091) clarifies the requirements, expectations, and procedures for evaluating the feasibility and performance of natural attenuation as a component of a cleanup action and provides general guidance on how to conduct such an evaluation.

This document (User's Manual; Ecology Pub. No. 05-09-091A) provides step-by-step instructions on how to use the methods incorporated as part of the Data Analysis Tool Package (two Microsoft Excel® Spreadsheets) to evaluate the feasibility and performance of natural attenuation. This document is intended for site managers and anyone who is contemplating using natural attenuation to clean up ground water contaminated with petroleum hydrocarbons. Persons using this Manual should be appropriately trained[1] in the performance of remedial actions and should exercise the same care and professional judgment as when performing any other remedial action. This User's Manual should be used in conjunction with the MTCA Cleanup Regulation and the other materials included as part of a natural attenuation guidance package.

The Data Analysis Tool Package (available separately) provides several different tools to evaluate the feasibility and performance of natural attenuation as a cleanup action under the MTCA Cleanup Regulation. This User's Manual describes what tools are included as part of the Data Analysis Tool Package and provides step-by-step instructions for:

- Chapter 2: general instructions such as how to obtain and use the Data Analysis Tool Package, and common error messages and troubleshooting tips;

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[1] *Most natural attenuation demonstration appears to fall within the scope of those activities that must be conducted by, or under the supervision of, a licensed professional engineer or geologist (Chapter 18.43 RCW and Chapter 18.220 RCW). Please consult with the appropriate licensing board for questions regarding these requirements.*

- Chapter 3 and Appendix A: brief description, function, and navigation of each calculation module;
- Chapter 4 and Appendix B: detailed explanation on how to enter data and interpret the output (calculation result) for each of the Modules included as part of the package, and associated mathematical equations and recommended decision criteria used;
- Appendix C: a table of properties (e.g., utilization factors, solubilities, molecular weight, etc.) of contaminants commonly found at petroleum-contaminated sites;
- Appendix D: simple fate and transport equations on how to calculate the basic *in situ* natural attenuation processes including natural biodegradation, advection, dispersion, and retardation of hazardous substances – several of these processes are defined in Section 1.7 of the guidance document (Ecology Pub. No. 05-09-091);
- Appendix E: a sample evaluation to assess the feasibility of natural attenuation with Data Analysis Tool Package "A"; and
- Appendix F: a definition and dimension of all symbols and abbreviations used in equations and tables of this document.

Use of the Data Analysis Tool Package (Workbook) may not be sufficient to evaluate the feasibility and performance of natural attenuation under the MTCA Cleanup Regulation. The Workbook is merely a computational tool and does not provide all information necessary to evaluate the feasibility and performance of natural attenuation. The user should have the appropriate background, training, and experience to use the Workbook and to analyze the results.

This User's Manual does not establish or modify regulatory requirements. While this User's Manual provides several useful evaluation tools to demonstrate compliance with regulatory requirements and makes recommendations regarding the appropriate use of those tools, persons do **not** need to use those specific tools and may use **alternative** tools to demonstrate **compliance**.

Chapter 2 General Instructions

2.1 Overview of Files

The zip archive file (*NAPetro10.exe*) contains two “Natural Attenuation Analysis Tool Packages for Petroleum-Contaminated Ground Water” in Microsoft (MS) Excel® XP (2002 version) format and general instructions in MS Word® XP (2002 version) format. The MS Excel® workbooks may be obtained by:

- Contacting Ecology (360-407-7224; cesg461@ecy.wa.gov) to obtain a compact disk (CD) containing the files; or
- Downloading the files from Ecology's Internet web site: *http://www.ecy.wa.gov/programs/tcp/policies/pol_main.html*

This User’s Manual provides general instructions on the use of the following two MS Excel® workbooks described below:

File Name	File Size (KB)	Description
Package A_ NAToolPetro10.xls	890	Tool Package A: Workbook for Natural Attenuation Analysis Tools without Ground Water Flow Model: Modules 1, 2, 3
Package B_ NAToolPetro10.xls	1,050	Tool Package B: Workbook for Natural Attenuation Analysis Tools with Ground Water Flow Model: Modules 4, 5, 6

2.2 Hardware and Software Requirements to Run the Natural Attenuation Analysis Package

Any hardware capable of operating MS Excel® XP (2002) will run the workbooks. A math coprocessor is not required, but is recommended. Modern processors may have the coprocessor included. Please note you can check your hardware configuration if you are using MS Windows® by “right-clicking” on “my computer” on the windows desktop and selecting “system information.” Some workbook routines require intensive numeric processing best handled by hardware with greater amounts of Random Access Memory (RAM) and Pentium-level processors. Additional **hardware** recommendations include:

- A CD-ROM drive, if you have received the workbook on CD;
- A hard disk drive with at least 40 MB of free disk space;
- A minimum of 64 megabytes of system memory (RAM);
- 486 DX or higher processor running at 66 MHz or faster;
- Any monitor supported by Windows, with video graphics array (VGA) or better resolution; and
- An 800 x 600 monitor resolution or higher.

Recommended software needed to run the workbook and associated functions is MS Excel® version 2002 (or XP version) for Windows. However, MS Excel® 2000 or earlier should be compatible with natural attenuation analysis packages. The software is implemented as an MS Excel® workbook, programmed in Visual Basic® and Visual Basic for Applications® (VBA), and requires MS Excel®. Both tool package workbooks use automatic procedures programmed in MS Visual Basic®. However, it should not be necessary to have Visual Basic® installed on your particular system to operate the workbook.

Visual Basic® routines included in the Package B workbook make references or "calls" to library or add-in functions that may or may not be installed on your particular computer or activated in your current MS Excel® application. Even if these elements are installed, the Visual Basic® routines need to be edited to provide the correct path for them. The Visual Basic® routine needs to know where they "are" on your particular computer's hard drive or network. The discussion under Section 2.4, below, describes how to check the status of these elements and make the appropriate modifications so that the Package B workbook can run without encountering errors.

Note: Workbooks (Data Analysis Tool package) are offered for use without warranty or support. They are made to work with MS Excel® 2002 and may not work properly with other applications, or with early versions of MS Excel®. It is recommended that you have no other files open in Excel when using these workbooks.

2.3 Installation of the Workbooks

Once the workbook is copied to your hard drive, several modifications and changes to your MS Excel® "add-in" components are required to allow the routines contained in the workbook to operate correctly. To install the workbook, follow these instructions:

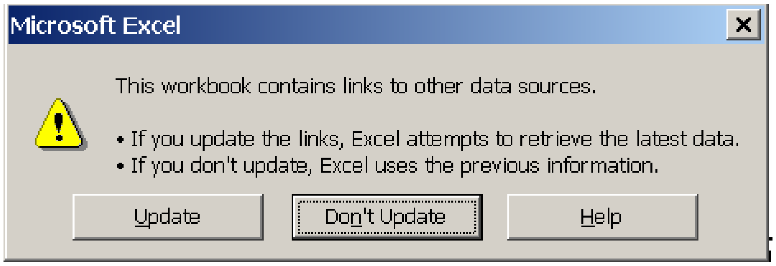
1. Copy the workbook file to the directory of choice.
2. Open Excel® and then open the file or simply double-click the workbook icon as you would do with any other Excel® file.
3. Click "**YES**" when you are asked about enabling the MACRO.
4. Click "**Don't Update**" when you are asked about updating links.
5. On the **Tools** menu, click **Add-Ins**. In the **Add-Ins available** box, select the check box next to "solver Add-In" and then click **OK**. If the add-in you want to use is not listed in the **Add-Ins available** box, click **Browse**, and then locate the add-in as explained in the section 2.4 of this document.
6. Save a working file under a user-specified (different from original) name. Use the END button when closing the file.

Note: Do not attempt to run the workbooks without saving the files to your hard drive. It may cause the error messages as described below, or the workbooks may not run properly.

2.4 Common Error Messages and Troubleshooting Tips

Opening error message "This Workbook contains links to other data source…" as shown or "#NAME?" is displayed in cell boxes:

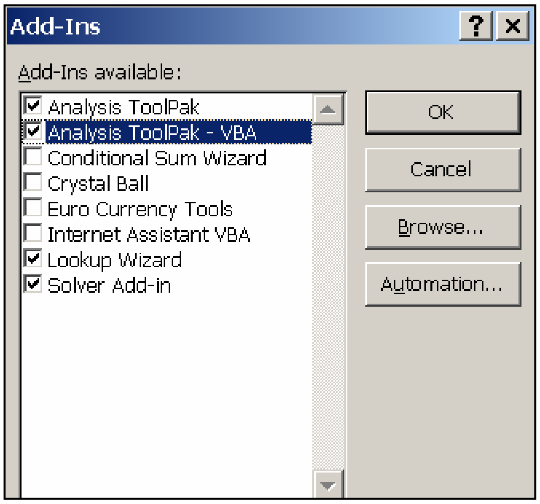
The most common cause of this problem is that necessary "add-ins" components are not added properly. Follow installation instructions described below:



This workbook contains links to other data sources.

- If you update the links, Excel attempts to retrieve the latest data.
- If you don't update, Excel uses the previous information.

1. Click "**Don't Update**" when you are asked about updating links.
2. On the **Tools** menu, click **Add-Ins**. In the **Add-Ins available** box, select the check box next to the add-in you want to load as shown to the right, and then click **OK**. If the add-in you want to use is not listed in the **Add-Ins available** box, click **Browse**, and then locate the add-in. If necessary, follow the instructions in the setup program. Or, you can reinstall an Excel® add-in by using the program that you used to install Excel®.



Add-Ins available:

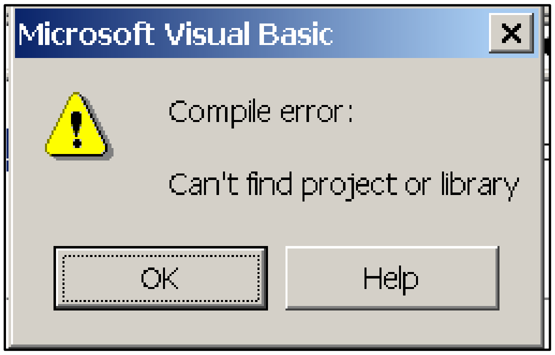
☑ Analysis ToolPak
☑ Analysis ToolPak - VBA
☐ Conditional Sum Wizard
☐ Crystal Ball
☐ Euro Currency Tools
☐ Internet Assistant VBA
☑ Lookup Wizard
☑ Solver Add-in

- ***Analysis ToolPak***
- ***Analysis ToolPak-VBA***
- ***Lookup Wizard***
- ***Solver Add-In***

Opening error message "Compile error: can't find project or library" or not executing the calculation:

It is possible that MS Visual Basic® may open with an error window that states ***"Compile error: Can't find project or library."*** If this is the case, it is likely that the Visual Basic® routines included in the workbook cannot locate one or both of the following function files that need to be present on your computer's hard drive to allow the workbook to perform correctly:

- ***LOOKUP.XLA***
- ***SOLVER.XLA***



Compile error:

Can't find project or library

This usually is caused by not having the **Solver Add-in** open and loaded. It is the user's responsibility to verify that these files are correctly loaded. To see if you have these files, use your file browser to search for them. Usually, these files are located in the Library folder contained in the Office folder. The file ***"SOLVER.XLA"*** probably is contained in a folder called ***"Solver"*** within the library folder. If you don't have these files, you may need to install one or both of them from your original MS Office® source disk. In order to establish a path to these files for the workbook, you may need to do the following:

1. In Visual Basic® (with the error window showing), click on [OK] in the error dialogue window to close it.
2. Click on [Run] in the main toolbar and select [Reset].
3. Click on [Tools] in the main toolbar and select [References].

A list of available references with checkmarks will appear for the workbook. Follow these instructions for each checked reference that is labeled as “MISSING” (you should repeat this procedure for each missing reference):

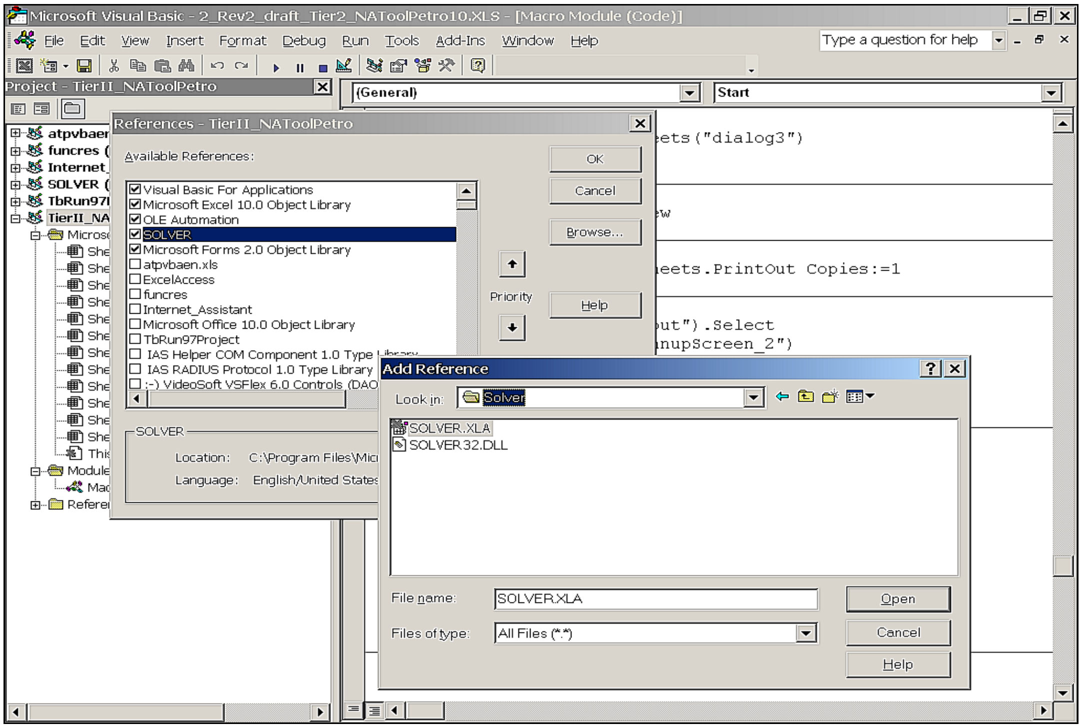
1. Highlight the file with your cursor (if it is not already highlighted).
2. Click on [Browse] at the right side of the dialog box.
3. Using the browser, locate the missing file (probably under Office/Library). Be sure to select “All Files” in the [Files of Type:]; scroll-down window so that all files in the particular folder will be displayed. If you still have trouble locating a particular file, you may right-click on “My Computer” on your desktop and select “Explorer” from the pop-up menu. Then fill in the appropriate file name to search for the location. To search for the missing file under MS Windows® 2000:

    a) Click **Start**, point to **Search**, and then click **For Files or Folders**.
    b) In **Search for files or folders named**, type all or parts of the missing file name you want to find.
    c) In **Look in**, click the drive, folder, or network you want to search.
    d) To specify additional search criteria, click **Search Options**, and then click one or more of the options to narrow your search.
    e) Click **Search Now**.

If the file is not located, you may need to install it from the source disk or check with your PC administrator. In most cases, you may be able to find the file "***SOLVER.XLA***" located in the following folder:

- “*C:\Program Files\Microsoft Office\Office10\Library\Solver*” for MS Excel® XP and 2002 versions
- “*C:\Program Files\Microsoft Office\Office\Library\Solver*” for MS Excel® 97 version

4. Once the file is located (be sure it’s the one with the “***xla***” extension), click on it (highlight it) and then click on the [Open] button. The window should return to the “Available References” list. The file should have a check-mark next to it. Repeat this process for each additional missing file.
5. Click [OK] to close the Available References window.
6. Click [File] in the main toolbar and select [Save]. Close Visual Basic® (this should return you to the MS Excel® workbook). Save the corrected Visual Basic® Routines under a new file name if necessary. Installation is now complete. Check by closing the workbook and re-opening in MS Excel®. It should open to the title sheet without any error messages.



Available References:

- ☑ Visual Basic For Applications
- ☑ Microsoft Excel 10.0 Object Library
- ☑ OLE Automation
- ☑ SOLVER
- ☑ Microsoft Forms 2.0 Object Library
- ☐ atpvbaen.xls
- ☐ ExcelAccess
- ☐ funcres
- ☐ Internet_Assistant
- ☐ Microsoft Office 10.0 Object Library
- ☐ TbRun97Project
- ☐ IAS Helper COM Component 1.0 Type Library
- ☐ IAS RADIUS Protocol 1.0 Type Library
- ☐ :-) VideoSoft VSFlex 6.0 Controls (DAO

SOLVER
Location: C:\Program Files\Mic
Language: English/United States

Look in: Solver

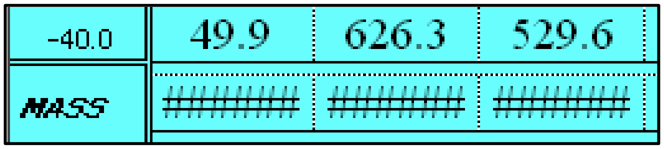
SOLVER.XLA
SOLVER32.DLL

File name: SOLVER.XLA
Files of type: All Files (*.*)

```
ets("dialog3")
w
eets.PrintOut Copies:=1
ut").Select
nupScreen_2")
```

Note: The macro within the workbook that calls the subroutines operated upon by "SOLVER" and/or "LOOKUP" does not know where to look on the hard drive: it only "looks" in the folder it is operating within, UNLESS the user establishes a path to these files for the workbook. If the instruction given above does not work, please copy three MS Excel® files (SOLVER.XLA, SOLVER32.DLL, and LOOKUP.DLL or equivalent files for a different version of MS Excel® 2000) into the same folder that contains the downloaded workbook.

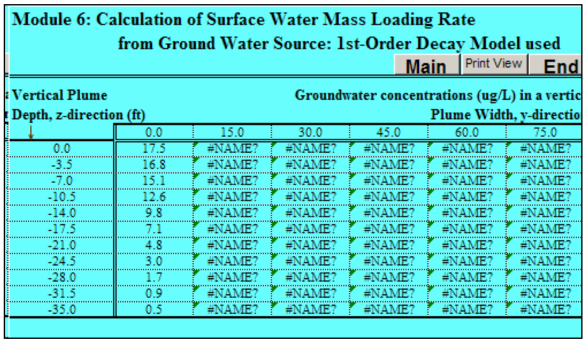
<u>"# # # #" is displayed in a number box</u>:
Display properties chosen by users are not compatible with the cell format originally designed for the value (e.g., the number is too big to fit into the cell window). To fix this problem, select the cell, pull down the format menu, select "Cells" and click on the "Number" tab. Change either the format, length of column, or the font size of the cell until the value is visible.



-40.0	49.9	626.3	529.6
MASS	#########	#########	#########

<u>"# DIV/0!" is displayed in a box</u>:
The most common cause of this problem is that some input data are missing. Double-check to make certain that all of the input cells required for your run have data in them.

<u>"#NAME?" is displayed in all cell boxes of the Calculation of Surface Water Mass Loading Rate</u>:
Refer to Section 2.3 (installation tip) of this User's Manual.



Module 6: Calculation of Surface Water Mass Loading Rate
from Ground Water Source: 1st-Order Decay Model used

Vertical Plume Depth, z-direction (ft)	Groundwater concentrations (ug/L) in a vertic Plume Width, y-directio					
↓	0.0	15.0	30.0	45.0	60.0	75.0
0.0	17.5	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-3.5	16.8	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-7.0	15.1	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-10.5	12.6	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-14.0	9.8	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-17.5	7.1	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-21.0	4.8	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-24.5	3.0	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-28.0	1.7	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-31.5	0.9	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?
-35.0	0.5	#NAME?	#NAME?	#NAME?	#NAME?	#NAME?

The buttons won't work:
Click on another cell or hit the enter/return key, and then click the buttons and they should work.

Text labels appear to be cut off:
On some monitor resolutions in MS Windows® some cell labels may appear cut off. This should affect only the screen display, and in most cases, printouts should not be affected.

Other potential error messages:
It is possible that you may receive other error messages when trying to open the workbooks. Be sure the MACROs are activated in order to use the tools properly. Some error messages may require you to refer to online help or the documentation of the host application. Check with your network operator or information technology specialist to be sure your MS Excel® application can accept MACROs operation and to address other host application-related errors.

Opening more than one workbook at a time:
It is not advisable to load and use more than one copy of the same workbook (either ***Package A*** or ***B***) at the same time.

Viewing the worksheets:
Some users may have a difficulty viewing worksheet numbers or text. To enlarge your view of a particular sheet, click on "View" in the main toolbar and select "Zoom." Choose a magnification that works best for your needs and save it as modified.

Resizing and rescaling the graph:
Users can manually resize the graph or rescale (e.g., from or to normal to log scale) the axis to make it look more meaningful by double-clicking on the graph and resizing and rescaling it. Refer to the MS Excel® user's manual.

2.5 Saving and Closing (exiting) the Workbook

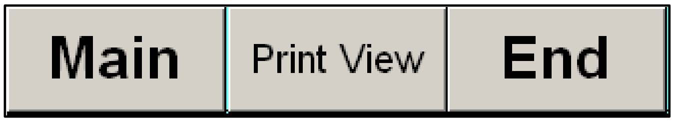
→ USE THE END BUTTON ←

Once an analysis is complete, it is good practice to print out a copy of the entire workbook for your records. You may also wish to save the workbook under a new name [FILE – SAVE AS].

Note: The workbook should be closed (exited) using the END button at the top of the sheet. Do not close the workbook using the typical means provided in Excel (i.e., [FILE-CLOSE] or clicking on the "X"). Using the END button allows the programmed routines in the workbook to return the Excel® toolbar displays and other format options to those you normally use. If you accidentally exit without using the END button, you can re-establish your toolbars by clicking on [VIEW-TOOLBARS] and selecting the toolbars you wish to use. You may also need to click on [TOOLS-OPTIONS] and make selections as appropriate to re-establish certain work area components. When you click on the END button, you will be prompted to save your work, and you can do so by answering [yes] and saving the file under a new file name. Otherwise, answer [no] and you will exit the workbook without saving any changes.

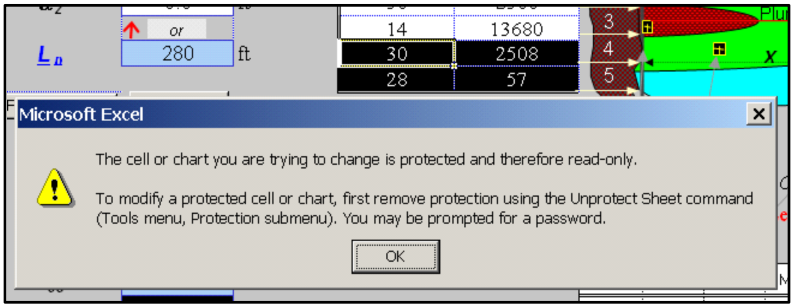
2.6 Preview, Printout, and Readability of Worksheet

The workbooks provide printing and reviewing capabilities for all input/output screens. Input/output worksheet prints on one page for most computer/printer configurations. The worksheet is designed at "1024 x 768" pixel screen resolution, making it more readable on new computer configurations. For older systems with lower resolution, simply changing the screen "zoom" level to a higher percent (or more) instead of lower percent will improve readability.



2.7 Security and Protection of Worksheet

The worksheets have been provided unlocked and unprotected. It therefore is critical that Ecology site managers are confident that the formulas used for calculations are accurate. Unfortunately, submittals could include printouts from worksheets that contain modified formulas, which could result in erroneous results. For this reason, the security on the workbooks can be increased by locking the worksheets.

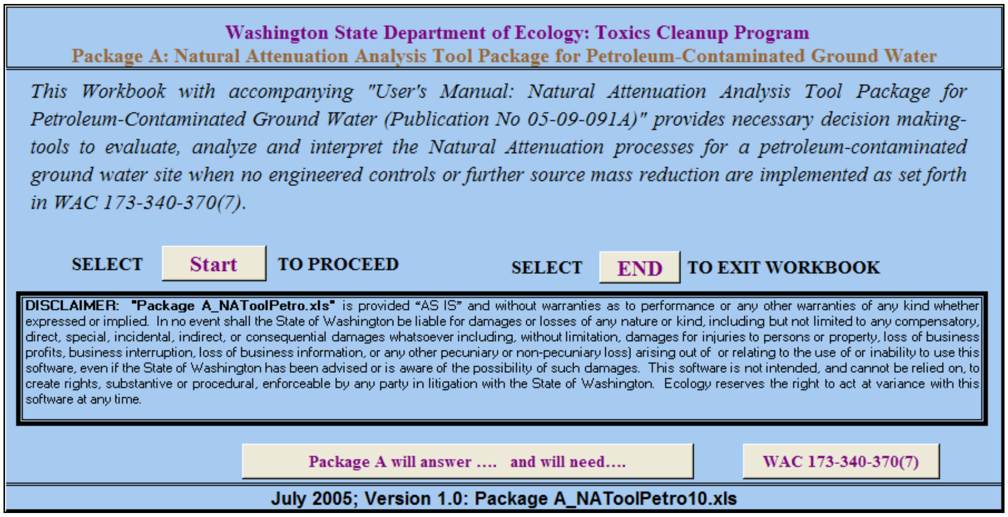


The cell or chart you are trying to change is protected and therefore read-only.

To modify a protected cell or chart, first remove protection using the Unprotect Sheet command (Tools menu, Protection submenu). You may be prompted for a password.

2.8 Accessing the Worksheet and Opening Title Screen

Once the workbook is successfully loaded into MS Excel®, the title sheet will appear. Be sure to enable the MACROs. To use the natural attenuation workbook tool, click on the START button (to exit, click on the END button). It is important to use the END button to exit the workbook so your previous default MS Excel® settings (toolbars, work-area format) are restored. Selecting the START button makes the Navigator appear on your screen (light blue background).



Washington State Department of Ecology: Toxics Cleanup Program
Package A: Natural Attenuation Analysis Tool Package for Petroleum-Contaminated Ground Water

This Workbook with accompanying "User's Manual: Natural Attenuation Analysis Tool Package for Petroleum-Contaminated Ground Water (Publication No 05-09-091A)" provides necessary decision making-tools to evaluate, analyze and interpret the Natural Attenuation processes for a petroleum-contaminated ground water site when no engineered controls or further source mass reduction are implemented as set forth in WAC 173-340-370(7).

DISCLAIMER: "Package A_NAToolPetro.xls" is provided "AS IS" and without warranties as to performance or any other warranties of any kind whether expressed or implied. In no event shall the State of Washington be liable for damages or losses of any nature or kind, including but not limited to any compensatory, direct, special, incidental, indirect, or consequential damages whatsoever including, without limitation, damages for injuries to persons or property, loss of business profits, business interruption, loss of business information, or any other pecuniary or non-pecuniary loss) arising out of or relating to the use of or inability to use this software, even if the State of Washington has been advised or is aware of the possibility of such damages. This software is not intended, and cannot be relied on, to create rights, substantive or procedural, enforceable by any party in litigation with the State of Washington. Ecology reserves the right to act at variance with this software at any time.

July 2005; Version 1.0: Package A_NAToolPetro10.xls

When this button Package B will answer.... and will need.... is selected, the following additional information that pertains in the tool package chosen will be provided:

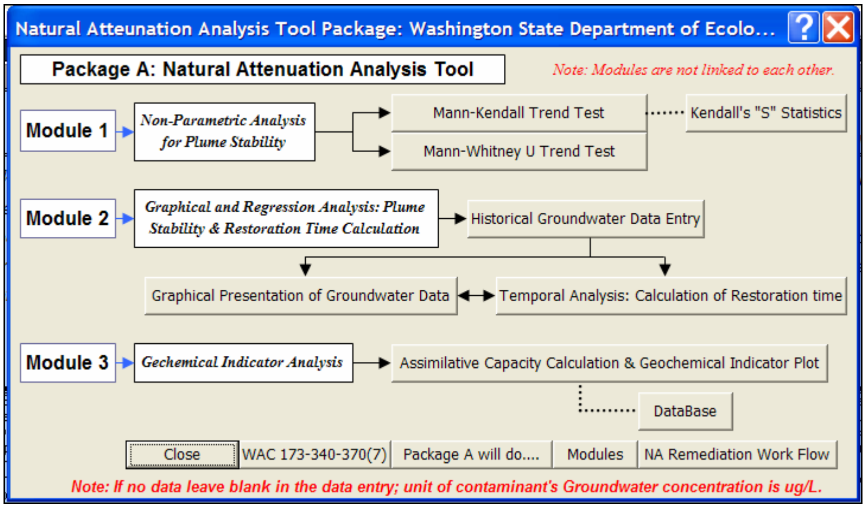
- Types of questions to be answered;
- Types of minimum data needed; and
- Types of calculations to be done.

Refer to Chapter 3 and Appendix B of this User's Manual for a detailed discussion.

2.9 Navigating to Different Modules in the Workbook

Each worksheet in the workbook contains a button labeled MAIN. This button can be used to go back to the navigation box shown below. Once you arrive at a particular sheet using the navigation box, you should click on the Close button (at bottom left) before continuing. When the START button is selected, the workbook loads a navigation box as shown below:

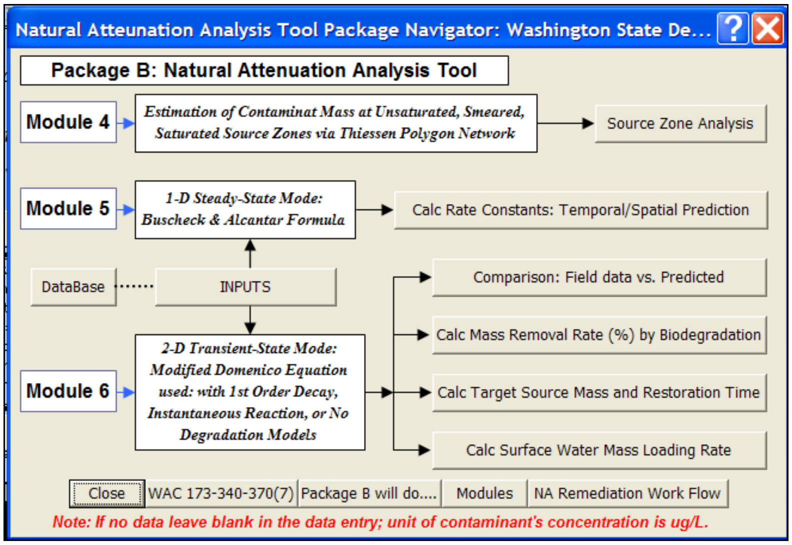
Package A



Note: Modules are not linked to each other.

Note: If no data leave blank in the data entry; unit of contaminant's Groundwater concentration is ug/L.

Package B



Note: If no data leave blank in the data entry; unit of contaminant's concentration is ug/L.

Additional buttons in the navigator are:

- Package A will do.... This button explains the functions of the tool package chosen, such as "types of questions to be answered, minimum data needed, and types of calculations to be conducted."
- Modules This button shows the functions of each module that is a part of the tool package. Refer to Appendix A of this User's Manual for details.
- NA Remediation Work Flow This button shows the generic remediation work flow that incorporates natural attenuation as a cleanup action at petroleum release sites.
- DataBase This button shows the supporting physical-chemical information and stoichiometric utilization factor used in the workbook calculations for petroleum-associated contaminants. There is some blank space available for the user-specified chemical that is a contaminant in the ground water at a site.
- WAC 173-340-370(7) This button shows the MTCA rule language associated with natural attenuation as a cleanup alternative (WAC 173-340-370(7)).

2.10 General Instructions on the Use of Worksheets

When a worksheet is first opened:
It contains example data such as the site name, site address, additional descriptions, names of monitoring well, dates of sampling, well concentrations, ground water elevations, and hydrogeological information, etc. The example data should be cleared, and new data should be entered. If new data entry causes an error message, you may have inadvertently attempted to delete/enter/edit cells that are not designed for data entry.

Do not change formulas or other information in cells with any colored background:
Note that only cells with a non-colored background are used for data entry. Usually, other colored cells in the worksheet are write-protected and cannot be modified. Do not try to change formulas or other information in cells with any colored background.

New unprotected worksheets:
If necessary, a whole blank unprotected worksheet can be created in each workbook so that the user can write custom code (or other calculations) for linking worksheets, etc.

Hidden and unhidden cells:
Most cells, rows, and columns are unhidden. The user should be able to "see" what is going on and formulae that are associated with the cell of concern. Contents of a cell can be inspected by placing the cursor on that cell.

To improve readability:
Some text that shows the calculation results are displayed in a different color, such as error messages and expanding trends. For example, undetermined trends are displayed in grey-colored text under Module 1 of the Natural Attenuation Analysis Tool Package.

To return to the navigator:
Click on MAIN in the upper either right or left corner of each worksheet to return to the navigator.

2.11 Header Information

In the rectangular (not-colored) box at the top of the worksheet, enter site name, site address, and detailed site description. Once an evaluation has been completed for a particular site, it is good practice to print out the results. Click on the Preview button to confirm that the proper header information appears on all printout worksheets. Remember to change the header information EACH TIME a new set of data is entered.

2.12 Entering Data for Inputs

All entries except header information must be numeric values:
A text entry at the data entry cell will cause a calculation error in the cells that they are associated with. This must be corrected or the workbook will not execute its calculations correctly.

Copying data from another worksheet for data entry cells:
Some users prefer to update and maintain a separate site data spreadsheet by copying data from that worksheet to paste into the Ecology-supplied natural attenuation worksheets. Generally, a "copy-and-paste" function is **not** recommended when doing this. Instead it is recommended that the "copy" function be used and not the "cut" function to copy data from the site data spreadsheet. If data is "cut" and pasted, there is a high probability that the formulae will be corrupted, whereas the "**copy"** function is much less likely to cause inaccurate results or an error message. When "pasting" data in MS Excel, please note that you may be pasting not just data, but other formulae, formats, comment, etc., from the original cells. To avoid this occurrence, use the "**paste special"** and select the button for "**values"** (rather than the default "all" button). Similarly, the practice of copying (or cutting) and pasting the entire worksheet into other worksheets or workbooks is **not** recommended, as there also is a high probability that the formulae will be corrupted and provide incorrect results.

Handling of non-detect values of the measured ground water contaminant concentration:

- Mann-Kendall Trend Test (under Module 1): To avoid biasing the Mann-Kendall test, the same value for all Non-Detect (ND) results must be entered in the spreadsheet for a given hazardous substance. This is to make sure that any identified trends are data trends and not trends of laboratory detection (or reporting) limits. Ecology recommends that the value that is entered for ND results be one-half of the detection (or reporting) limit from the round with the highest detection limit for that hazardous substance. For example, if the results for Benzene were <2.0, <2.0, <4.0 and <4.0 ug/L, enter 2.0, 2.0, 2.0 and 2.0 into the Module 1 worksheet for "Mann-Kendall Trend Test" instead of 1.0, 1.0, 2.0 and 2.0. This recommendation is specific only to the Mann-Kendall test.

- Mann-Whitney U Trend Test (under Module 1): Use "Zero" for Non-Detect values. This recommendation is specific only to the Mann-Whitney U test.

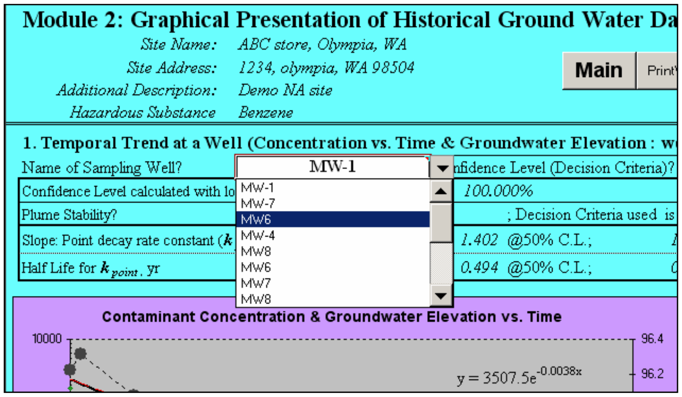
For all other Modules (under Module 2 through 6) follow the requirements in WAC 173-340-720(9), restated as follows: For the values for ground water contaminant and geochemical indicator concentration measurement below the method detection limit, substitute one-half the method detection limit. For the values for ground water measurement above the method detection limit but below the practical quantitation limit, substitute the method detection limit. However, for hazardous substances or petroleum fractions that have never been detected in any soil or ground water sample at a site and where these substances are not suspected of being present at the site based on site history and other knowledge enter "zero" for these hazardous substances or petroleum fractions for further calculation.

Unit of contaminant's concentration:
The data must be entered in consistent units. Unit of a contaminant for both tool packages (A and B) is ***μg/L*** for ground water and ***mg/kg*** for soil media throughout all calculation procedures unless stated otherwise.

Confidence levels (decision criteria):
Ecology generally recommends analyzing all natural attenuation process at 85% confidence level for both Tool Packages A and B. For the values of confidence levels as decision-making criteria, use a fractional form with decimal point. For instance, enter either "**0.85**" or "**85**" for 85% confidence level.

Leaving blank if no data:
Never enter zero value for data that are not available. **Leave blank if there are no data available.**

Displaying a list box to display available alternatives:
A list box or drop-down as shown on the right scrolls to display available alternatives. Select the choice you want to enter the data and click the down arrow to the side of the list box. Enter data in a cell from a list selected.



Module 2: Graphical Presentation of Historical Ground Water Da

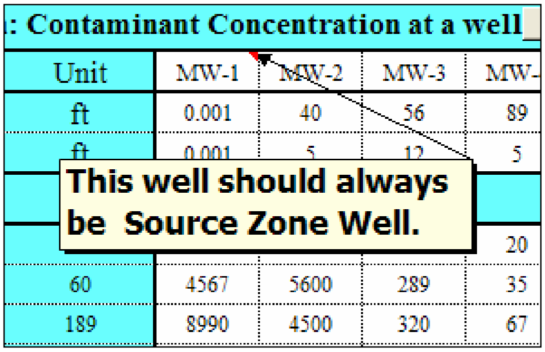
Site Name: ABC store, Olympia, WA
Site Address: 1234, olympia, WA 98504
Additional Description: Demo NA site
Hazardous Substance Benzene

1. Temporal Trend at a Well (Concentration vs. Time & Groundwater Elevation : w

Name of Sampling Well? MW-1
nfidence Level (Decision Criteria)?
Confidence Level calculated with lo 100.000%
Plume Stability? ; Decision Criteria used is
Slope: Point decay rate constant (k 1.402 @50% C.L.;
Half Life for k_{point}, yr 0.494 @50% C.L.;

2.13 Display or Hide Comments on Cells and Comments Indicators

When you rest the pointer over the cells that have a red-colored comment indicator located on the right upper-corner as shown below, the cells will show specific comments (notes) on the particular cell that users have to be aware of before entering the data. To hide or display comments and/or indicators throughout the workbook, click **Options** on the **Tools** menu and then click the **View** tab. To show indicators but display comments only when you rest the pointer over their cells, click **Comment** indicator only. To hide both comments and indicators throughout the workbook, click **None** under Comments.



: Contaminant Concentration at a well

Unit	MW-1	MW-2	MW-3	MW-
ft	0.001	40	56	89
ft	0.001	5	12	5
				20
60	4567	5600	289	35
189	8990	4500	320	67

This well should always be Source Zone Well.

2.14 Equations and Associated Symbols used for Calculation

Definitions and units of symbols/abbreviations used in equations shown throughout this User's Manual and natural attenuation analysis package worksheets can be found in the Appendix F (Symbols and Abbreviations) of the guidance document (Pub. No. 05-09-091A) unless stated otherwise.

Note: For additional information on Tool Package B natural attenuation analysis with Domenico's analytical solution, refer to "User's Manual Version 1.4: BIOSCREEN Natural Attenuation Decision Support System" (Newell et al., 1997[2]).

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[2] Newell, C.J., Gonzales, J., and McLeod, R., 1997, BIOSCREEN: Natural Attenuation Decision Support System User's Manual, Versions 1.4 and 1.3, EPA/600/R-96/087, US EPA, Office of Research and Development, Washington D.C., July, 1997.

Chapter 3 Calculation Modules

Brief descriptions and functions of each calculation module are depicted in Appendix A of this User's Manual. The following lists the details on the functionality of each package.

3.1 Package A Natural Attenuation Analysis Tool (Modules 1, 2, and 3)

Package A analysis tool will answer the following questions:

- Is the plume shrinking, expanding, stable, or undetermined (with graphical and regression analysis, and non-parametric statistical analysis)?
- How long (an average and a range) will it take until the ground water concentration at each well reaches a target level as a result of natural attenuation processes?
- Is the site able to clearly (and qualitatively) demonstrate enough evidence of biodegradation (assimilative capacity)?
- Is the concentration of ground water impacted (systematically) by ground water elevation fluctuations?

Package A analysis tool will require the following minimum data:

- At least the following historical ground water contaminant concentrations that are above detection limit and elevation data are required
  - Mann-Kendall test: four or more sampling rounds in four or more consecutive wells
  - Mann-Whitney U-test: eight sampling rounds in four or more consecutive wells
  - Graphical and regression analysis: four or more sampling rounds in four or more consecutive wells
- Target ground water concentration at each well
- Average concentration for geochemical indicators for four or more consecutive wells including up-gradient and down-gradient wells
- Location (2-D) of all monitoring wells

Package A analysis tool will conduct the following:

- Non-parametric statistical tests for plume stability at each well
  - Mann-Kendall test
  - Mann-Whitney U-test
- Graphical presentation of historical ground water data
  - Plot of temporal ground water analytical and elevation data vs. time to assess the plume status and the impact of ground water elevation fluctuation on contaminant concentrations at each well
  - Plot of spatial ground water analytical data vs. distance (for multiple wells) to assess the overall plume status
- Evaluation of geochemical indicators
  - Estimate of expressed assimilative capacity at multiple wells
  - Simultaneous plot of concentrations of contaminant and geochemical indicators vs. distance (at multiple wells) to demonstrate biodegradation clearly
- Temporal trend (regression) analysis at each well

- ➢ Estimate of an average and a range of (k_{point}) point decay rate (1^{st}-order) constant for both the best-fit and a given one-tailed confidence level at each well
- ➢ Temporal prediction at each well location under a given confidence level
- ➢ Estimate of an average and a range (under a given confidence level) of restoration time to reach the cleanup goal at each well
- ➢ Calculation of the correlation coefficient and confidence level (with the Pearson's correlation coefficient) of log-linear regression analysis (for a plot of concentration vs. time at each well)

3.2 Package B Natural Attenuation Analysis Tool (Modules 4, 5, and 6)

Package B is modified from BIOSCREEN: Version 1.4 (Newell et al., 1997[2]). Details of modification made can be found in the Section of 4.7 of this document.

Package B analysis tool will answer the following questions:

- How far will the dissolved plume extend if no engineered controls or further source zone mass reduction measures are implemented?
- How long will it take until the ground water concentration will reach a target level at a receptor location by the natural attenuation processes?
- Under the natural attenuation processes, how much of the mass (%) in the plume can be removed by biodegradation alone?
- How much source zone mass reduction (or concentration reduction) at the source will be necessary to reach a target level at a receptor location under the given restoration time by natural attenuation processes?

Package B analysis tool will require the following minimum data:

- Under 1-D (transformed from 2-D) steady-state assumption
  - ➢ Basic site-specific hydrogeology data (seepage velocity, longitudinal [x-direction] dispersivity, retardation factor)
  - ➢ The most recent representative average contaminant concentrations that are well above detection limit in four or more consecutive wells sampled over four or more sampling rounds
  - ➢ Location (2-D) of all monitoring wells being used for the natural attenuation calculation
  - ➢ Target ground water concentration and location of "point of compliance"
- Under 2-D transient-state assumption:
  - ➢ Contaminant source dimension (width and depth) and mass
  - ➢ Basic site-specific hydrogeology data (seepage velocity, longitudinal [x-direction] dispersivity, retardation factor)
  - ➢ Contaminant release time
  - ➢ The most recent representative average contaminant concentrations that are well above the detection limit in four or more consecutive wells sampled over four or more sampling rounds
  - ➢ Average concentration for geochemical indicators for overall plume (for instantaneous reaction model only)
  - ➢ Location (2-D) of all monitoring wells being used for the natural attenuation calculation
  - ➢ Target ground water concentration and location of "point of compliance"

Package B analysis tool will conduct the following calculations:

- Estimate of source mass from sampling data: for unsaturated, smear, and dissolved zones
- Under 1-D (transformed from 2-D): steady state/continuous source assumption for only stable plume (with Buscheck and Alcantar model: see footnote on page 33 of this User's Manual)
  - ➢ Plot of the concentration vs. distance
  - ➢ Estimate of an average and a range of (λ) biodegradation rate constant
  - ➢ Estimate of an average and a range of (k) bulk attenuation rate (1st-order) constant under steady state (stable plume)
  - ➢ Estimate of a percent mass removal rate by biodegradation alone
  - ➢ Temporal and spatial prediction as a function of time and well location
  - ➢ Estimate of a target source concentration in order to reach a target level at a receptor location under given restoration time
- Under 2-D; transient state (with modified Domenico model) for shrinking and stable (or any type) plumes:
  - ➢ Estimate of a biodegradation rate constant (λ) by calibration via chi-square statistics for best-fit to the normalized concentration of consecutive multiple wells by 1st-order decay model
  - ➢ Estimate of a percent mass removal rate by biodegradation alone with 1st-order decay model and instantaneous reaction model (via the calculation of mass flux)
  - ➢ Estimate of a temporal/spatial prediction at a receptor location by 1st-order decay model and instantaneous reaction model
  - ➢ Estimate of a plume stabilization time (half time to reach the steady state) at a receptor location
  - ➢ Estimate of a restoration time to reach a target level at a receptor location by 1st-order decay model and instantaneous reaction model
  - ➢ Estimate of a target source mass amount (amount of mass that should be removed from the current source zone) in order to reach a target level at a receptor location under a given restoration time by 1st-order decay model and instantaneous reaction model
  - ➢ Estimate of a contaminant mass loading rate (as a function of x-distance and time) to the adjacent surface water body by 1st-order decay model

Chapter 4 Data Entry and Interpretation of Output

The Natural Attenuation Analysis Tool Package requires entering data to evaluate the natural attenuation process. This chapter explains step-by-step how to enter the data, operate, and interpret the natural attenuation process with each worksheet. The natural attenuation analysis tools must be run in the order of the number assigned for each action as below.

Note that the number assigned for each action/evaluation activity also identifies the exact location of worksheets that are depicted in Appendix B of this User's Manual.

4.1 Module 1: Non-Parametric Analysis for Plume Stability Test

Both non-parametric statistical test worksheets contained in Module 1 are modified from the State of Wisconsin (2001[3]).

Mann-Kendall Trend Test for Plume Stability of Each Well (Non-parametric Statistical Test): To use the Mann-Kendall Trend Test worksheet, provide at least four rounds and not more than 16 rounds of data. The Mann-Kendall Trend Test is not valid for data that exhibit strong seasonal behavior. Use consistent units. The worksheet is set up for multiple contaminants for a well (or for multiple wells for a contaminant). The generic templates, when first loaded include the contaminants that are most applicable at most gasoline sites, but different contaminants may be entered instead. See Figure B.1.1 of this User's Manual.

1. Enter the logistical information: descriptive text for the identification of a particular site including site name, address, and any additional information.
2. Enter the name of well sampled: all ground water data (sampling dates, name of contaminants, and concentrations of contaminants) to be entered that are associated with this designated well.
3. Enter the level of confidence to be used as decision criteria for Mann-Kendall trend Test: this criterion will be used to define the plume status. Ecology recommends using 85% as the default decision criterion. Any data set lower than this decision criterion will be considered as either a stable plume or undetermined, depending upon the Coefficient of Variation (CV) calculation. As a simple test, the Coefficient of Variation can assess the scatter in the data:

$$CV = \frac{S\tan dardDeviation}{ArthmeticMean} \qquad \text{(Eq. 4.1)}$$

4. Enter the sampling dates: most recent date is entered last. The date format is "03/24/03." Dates that are not consecutive will show an error message of "DATE ERR" and will not display the test results properly. To use the Mann-Kendall Trend Test worksheet; provide at least four rounds and not more than 16 rounds of data that is not seasonally affected.
5. Enter the name of contaminants for non-parametric test of plume status associated with well location specified.

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[3] State of Wisconsin, 2001, Department of Natural Resources, Remediation and Redevelopment Program, Form 4400-215 & Form 4400-216.

6. Enter the ground water contaminant concentrations that are associated with the designated well and sampling dates.
7. A level of confidence is calculated for the specific data set entered above: this is determined from the Mann-Kendall's "S" statistics table (see the Kendall's S-Statistics table in Figure B.1.2 of this User's Manual) based on number of sampling rounds (n) and "S" value below.
8. Final determination of the plume status: Table 4.1 below explains how to determine the plume status under Mann-Kendall Trend Test.

Table 4.1. Mann-Kendall Trend Test (for each well)

Status of Plume	Decision Criteria			
	CL_{calc}	Sign of "S" value	CV	Number of sampling rounds
Shrinking Plume	$> CL_{DecisionCriteria}$	Negative	NA	>4
Expanding Plume	$> CL_{DecisionCriteria}$	Positive	NA	>4
Stable Plume	$< CL_{DecisionCriteria}$	NA	<=1	>4
Undetermined	$< CL_{DecisionCriteria}$	NA	>1	NA

Note: CL_{calc}*: Confidence Level calculated for specific data given*
$CL_{DecisionCriteria}$*: Confidence Level predetermined as a decision criterion*
CV: Coefficient of Variation to account the magnitude of scatter in the data
NA: Not Applicable

9. This is a criterion to define whether the plume is stable by checking whether the Coefficient of Variation calculated is lower than "one".
10. The computed "S" value: this value is used for calculating confidence level.
11. The number of sampling rounds, the average concentration, and the standard deviation of the data set entered above is computed.
12. The Coefficient of Variation for the data set entered above is computed for checking the magnitude of scatter in the data to further define the stable plume.
13. "Blank if no errors found": this row displays an error sign. Dates that are not consecutive will show an error message and will not display the test results. When there are less than four rounds of data entered, an "ERROR" message of "n<4" is displayed. If text or a zero or a negative number is inadvertently entered, the "ERROR" message is also displayed. Note that to avoid an error message the date must be entered before sample results collected on that date are entered.
14. Select the name of the contaminant from a drop-down menu to plot the concentration vs. sampling date and visually observe the plume status.

Mann-Whitney U Trend Test for Plume Stability for Each Well (Non-parametric Statistical Test):

The Mann-Whitney U Trend Test is applicable to data that may or may not exhibit seasonal behavior. Use consistent units. The worksheet is set up for multiple contaminants for a well. The generic templates, when first loaded, include the contaminants that are most applicable at most gasoline sites, but different contaminants may be entered instead. See Figure B.1.3 of this User's Manual.

1. Enter the logistical information: descriptive text for the identification of a particular site including site name, address, and any additional information.
2. Enter the name of the well sampled for the evaluation of the plume status.
3. Enter the name of the contaminants for the non-parametric test of plume status that is associated with the well location specified previously.
4. Enter the sampling dates that the contaminants were sampled. The most recent date is entered last. The format is "03/24/03." Dates that are not consecutive will show an error message of "DATE ERR" and will not display the test results. Enter the most recent eight (8) consecutive quarterly or semi-annual sampling events for each contaminant that has exceeded the method detection limits.
5. "D_n-D_{n-1}": A period of time (days) passed after previous sampling round: to be used to determine the sampling frequency.
6. Enter the ground water contaminant concentrations that are associated with the designated well and sampling dates.
7. "U" statistic is calculated to determine plume stability.
8. The status of the plume is defined. "U" statistic is interpreted below to define the stability of the plume. For two groups of four samples, at a fixed confidence level of 90%, the stability of the plume is interpreted as shown in Table 4.2:

Table 4.2. Mann-Whitney U Trend Test (for each well)

Status of Plume	Decision Criteria (@ 90% Confidence Level)	
	U statistics	Number of sampling rounds
Shrinking Plume	≤ 3	> 8
Expanding Plume	≥ 13	> 8
Undetermined	Between 4 and 12	< 8

9. This row displays an error sign. When less than eight rounds of data are entered, if there are no text entries and no negative values, instead of getting an "ERROR" message, a "n<8" message will appear. If text or a negative number is inadvertently entered, the "ERROR" message is displayed. Thus, during data entry, an "ERROR" message is displayed only when there actually is an error.
10. This row displays an error sign associated with entering the sampling dates.
11. Pick a contaminant name from a drop-down menu to plot the concentration vs. sampling date and visually observe the plume status.

4.2 Module 2: Graphical and Regression Analysis for Plume Stability & Restoration Time Calculation

Inputs: Enter Historical Ground Water Data:
See Figure B.2.1 of this User's Manual.

1. Enter the logistical information: descriptive text for the identification of a particular site including site name, address, and any additional information.
2. Enter the name of the contaminant whose data will be analyzed and evaluated in two follow-up worksheets ("Temporal Analysis…." and "Graphical Presentation of …").

3. Enter the sampling dates that the contaminant was sampled. Most recent date is entered last. The date format is "03/24/03." The worksheet can handle up to 20 rounds of sampling events.
4. Enter the name of the well sampled: the most distant well from the source zone is entered last.
5. Enter the down-gradient distance (plume centerline: x-direction): the centerline distance between the monitoring location and the center of source zone. This parameter should be measured along the centerline of the plume as indicated on the diagram at the right top corner of the worksheet. For a discussion of detailed methodology on how to determine a direction (plume centerline) of ground water flow, refer to page 31 of this User's Manual.
6. Enter the off-centerline distance (y-direction): the perpendicular distance between the monitoring point and the plume centerline. This parameter should be measured from the centerline of the plume as indicated on the diagram located at the right top corner of the worksheet.
7. NOTE: Data previously entered can be cleared by pressing the "clear" button for each new dataset entry. Note that once cleared, data cleared will be deleted permanently and <u>won't be restored</u>.
8. A period of time (days) passed after the first sampling round is automatically calculated: to be used to calculate the sampling time.
9. Enter the measured concentrations of the contaminant that is associated with the designated wells and sampling dates.
10. Values of average, maximum, and minimum concentrations entered for each well location sampled are calculated to show the range of contaminant concentrations.
11. Enter ground water elevation data associated with the sampling locations and sampling dates.

<u>Temporal Analysis: concentration of contaminant vs. time (regression analysis for each well):</u> See Figure B.2.2 of this User's Manual. A linear regression analysis between log concentrations of the contaminant selected vs. time is conducted for a selected sampling location, and a statistical inference is made on this worksheet. Refer to Triola[4] (1997) for a detailed discussion of confidence level for linear regression analysis using a Pearson Correlation coefficient to determine whether there is sufficient evidence to conclude that there is a linear correlation between sampling time and the log of contaminant concentration at a designated well.

The worksheet will conduct the Student's t-test for the slope (computed by log-linear regression technique) of log concentration vs. time equal to "zero" for each well. That is, the worksheet performs Student's t-test on the slope of the log-linear regression line, with the **null hypothesis** that the **slope equals zero**. The confidence level attained for the t-test on the slope is compared to the predetermined level of confidence as a decision criterion to see if this slope is not statistically discernible from zero at the predetermined level of significance chosen by the user.

Note: The null hypothesis is that the slope on the log-linear regression line equals zero.

As there is natural scatter in most long-term monitoring data, there is uncertainty in the estimate of the point decay rate constant (k_{point}) and in the projected restoration time frame to achieve cleanup goals for that monitoring well. To account for this uncertainty, confidence intervals are calculated for each estimate of the point decay rate at a predetermined level of confidence. The

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[4] Triola, M., 1997, Elementary Statistics, see Chapter 9 - Correlation and Regression: pp. 476-501, 7th Edition, Addison-Wesley Inc.

level of confidence is the probability that the true rate (or a project restoration time) is contained within the calculated confidence interval. Refer to the US EPA's recent document (Newell et al., 2002[5] and US EPA, 2005[6]) for the discussion of uncertainty in rate calculations. Refer to a statistical textbook such as Lyman, 1999[7]; Devore and Peck, 2001[8], for a detailed calculation of confidence intervals (lower boundary) for a slope (a point decay rate constant) at a predetermined level of confidence.

1. Logistical information is carried over from the worksheet of "Inputs: Enter Historical Ground Water Data".
2. The name of contaminant to be evaluated is displayed.
3. Enter the level of confidence to be used as a decision criterion for a log-linear regression analysis. Ecology recommends using a value of 85% as a default. This criterion will be used for dual objectives in this worksheet, as below:

    - **To determine whether there is sufficient evidence to conclude that there is a linear correlation between sampling time and log contaminant concentration at a designated well.**
    - **To estimate the boundary value of slope (calculated with log-linear regression analysis) and consequent calculations for prediction of plume behavior.**

4. Enter a cleanup level for a selected well location to estimate the projected restoration time, if any.
5. Projected restoration times (time to reach the criterion) on average and lower boundary estimate with a predetermined level of confidence to reach the cleanup goal are displayed for a designated well.
6. Enter a specific date when the projected contaminant concentration is being calculated for a designated monitoring well.
7. Projected contaminant concentrations on average and boundary estimated with a predetermined level of confidence are calculated on a selected well.
8. The coefficient of determination (r^2), correlation coefficient (***r***), and a number (***n***) of ground water contaminant data used for a log-linear regression are calculated for a given set of ground water contaminant data for a selected well. The value of "***r***" must always be between -1 and +1. "***r***" measures the strength of a linear relationship between the sampling time and log concentration of contaminant. For a shrinking plume, the sign of "***r***" should be negative (inverse relationship). Both "***r***" and "***n***" are used to calculate the confidence level that is used to determine whether there is sufficient evidence to conclude that there is a linear correlation between sampling time and log contaminant concentration at a designated well.
9. The confidence level is calculated using the Pearson Correlation coefficient as explained above.

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[5] Newell, C.J., Rifai, H.S., Wilson, J.T., Connor, J.A., Aziz, J.A., and Suarez, M.P., 2002, Calculation and Use of First-Order Rate Constants for Monitored Natural Attenuation, US EPA Groundwater Issue Paper, EPA/540/S02/500, http://www.epa.gov/ada/pubs/issue/540S02500.html

[6] US EPA, 2005, Monitored Natural Attenuation of MTBE as a Risk Management Option at Leaking Underground Storage Tank Sites, EPA/600/R-04/1790, January 2005.

[7] Lyman, O. and Longnecker, M., 1999, An Introduction to Statistical methods and Data Analysis, Chapter 9 - Inferences Related to Linear Regression and Correlation, 5th edition, PWS-KENT Publishing company.

[8] Devore, J. and Peck R., 2001, Statistics: The Exploration and Analysis of Data, Chapter 13- Simple Linear Regression and Correlation: Inferential Methods, 4th Edition, Duxbury Product.

10. A decision on the statistical significance of log-linear regression is conducted. Confidence level (#9) calculated previously should be higher than the decision criteria (#3) previously determined in order to support a significant log-linear correlation between log-concentration vs. time.
11. Final determination of the plume status for each well: Table 4.3 explains how to determine the plume status with log-linear regression analysis. The plume can be defined as stable by checking if the Coefficient of Variation is less than one.

Table 4.3. Plume Stability Test with Regression Analysis (for each well)

Status of Plume	Decision Criteria			
	CL_{calc}	Sign of “r” value	CV	Number of sampling rounds
Shrinking Plume	$> CL_{DecisionCriteria}$	Negative	NA	>4
Expanding Plume	$> CL_{DecisionCriteria}$	Positive	NA	>4
Stable Plume	$< CL_{DecisionCriteria}$	NA	<=1	>4
Undetermined	$< CL_{DecisionCriteria}$	NA	>1	NA

Note: CL_{calc}: *Confidence Level calculated for a specific data set given*
$CL_{DecisionCriteria}$: *Confidence Level predetermined as a decision criterion*
CV: Coefficient of Variation to account the magnitude of scatter in the data
NA: Not Applicable

12. An average point decay rate constant (k_{point}) and half-life are calculated for a well.
13. A point decay rate constant and half life are calculated at a predetermined confidence level. An example interpretation of the temporal analysis result for “MW-1” is presented in Appendix B (Figure B.2.2) of this User’s Manual and is shown on Table 4.4:

Table 4.4. Examples of Regression Results

1. Level of Confidence (Decision Criteria)?			
2. Prediction: Calculation of Restoration Time and Predicted			
Well Location			**MW-1**
A. Cleanup Level (Criterion) to be achieved?		ug/L	100
A.1 Average (@50% CL[1] best-fitting values)			
Time to reach the criterion		yr	21.23
Date when the Criterion to be achieved		date	5/29/14
A.2 Boundary (@85% CL)			
Time to reach the criterion[2]		yr	27.02
Date when the Criterion to be achieved		date	3/13/20
B Date of Prediction?		date	5/16/09
B.1 Average conc predicted (@50% CL)		ug/L	282.56
B.2 Boundary conc predicted (@85% CL)		ug/L	577.75
3. Log-Linear Regression Results			
Coefficient of Determination	r^2		0.699
Correlation Coefficient	r		-0.836
Number of data points	n		13
4. Statistical Inference on the Slope of the Log-Linear Regres			
One-tailed Confidence Level calculated, %			99.963%
Sufficient evidence to support that the slope of the regression line is significantly different from zero?			YES!
Coefficient of Variation?			NA
Plume Stability?			Shrinking
5. Calculation of Point Decay Rate Constant (k_{point})			
Slope: Point decay rate constant (k_{point})	@50% CL	yr^{-1}	0.206
	@85% CL	yr^{-1}	0.162
Half Life for (k_{point})	@50% CL	yr	3.364
	@85% CL	yr	4.282

Note: The interpretation of Table 4.4 is as follows:

- *There is sufficient evidence to support a significant linear correlation (@ 99.9%) between sampling time and log concentration of Benzene at MW-1. In fact, the benzene plume at this well is found to be shrinking.*
- *On average (@ 50% confidence level), the estimated point decay rate constant (k_{point}) of Benzene is 0.21 per year (or half-life is 3.4 years), which requires 21 years to reach the cleanup goal of 100 ug/L. The predicted concentration at the projected date of 5/16/09 will be 283ug/L.*
- *At 85% confidence level, the lower boundary of confidence interval of point decay rate constant (k_{point}) of benzene is 0.16 per year (or half-life is 4.3 years). The upper bound of the time expected to reach the cleanup goal of 100 ug/L is 27 years. And the predicted concentration at the projected date of 5/16/09 will be 578 ug/L. This means that the length of time that will actually be required to achieve cleanup is estimated to be no more than 27 years at an 85% level of confidence.*

Graphical Presentation of Historical Ground Water Data for Each Well:
See Figure B.2.3 of this User's Manual.

1. Logistical information is carried over from the worksheet of "Inputs: Enter Historical Ground water Data".
2. The name of the contaminant selected for the evaluation is displayed.
3. Select the location of the monitoring point from the drop-down menu that is listed in the worksheet entitled "Inputs: Enter Historical Ground water Data".
4. Enter the level of confidence to be used as the decision criterion. Ecology recommends a value of 85% as a default.
5. The confidence level on the slope of the log-linear regression line for contaminant concentrations is calculated using the Pearson Correlation coefficient to see a significant evidence for log-linear correlation between concentrations vs. time at a selected well. Here, the status of the plume at a selected well is also defined at the predetermined level of confidence.
6. Average point decay rate constant (slope) and a point decay rate constant at a predetermined confidence level for the selected well are displayed.
7. The contaminant concentration and water elevation of a well vs. time is plotted simultaneously. The log-linear regression result of concentration vs. sampling time is displayed.
8. The contaminant concentration is plotted against its associated ground water elevation data.
9. Select up to six rounds of multiple sampling dates to visually examine the overall behavior of the contaminant plume as a function of sampling dates and projected plume centerline distance.
10. A plot of contaminant concentration (or log concentration) vs. distance down-gradient for a monitoring well over multiple sampling events is displayed. Historical ground water data are used to demonstrate a general trend of stable, decreasing, or expanding contaminant concentrations over time and along the plume centerline distance away from the source. The location of sampling wells expressed in terms of distance in x and y-direction is converted to the projected centerline distance from source as explained in Module 5 (see page 36 of this User's Manual).

4.3 Module 3: Evaluation of Geochemical Indicators

Assimilative Capacity Calculation and Geochemical Indicator Plot:
See Figure B.3 of this User's Manual.

1. Enter the logistical information: descriptive text for the identification of a particular site including site name, address, and any additional information.
2. Locate monitoring wells and enter the approximate plume centerline distance from the source. The distance for the "source well" has to be "zero".
3. Select a user-specified contaminant by using the drop-down menu. If the name of the contaminant is not displayed at the drop-down menu, go to the database (Refer to Appendix C of this User's Manual) via the Navigator by pressing the MAIN button, and create the name of the contaminant and its associated utilization factors associated with each geochemical indicator.

4. Enter representative up-gradient contaminant concentrations that are available at the site at each monitoring point.
5. Enter representative source contaminant concentration.
6. Enter representative down-gradient contaminant concentrations that are available at the site at each monitoring point.
7. Enter the representative background level (field measured concentration) for geochemical indicators.
8. Enter the representative levels (field measured concentrations) for geochemical indicators typical of the overall ground water plume.
9. Pick a name of a contaminant from the drop-down menu to calculate the expressed assimilative capacity.
10. The spreadsheet will display utilization factors assigned (from the database) for the previously selected contaminants.
11. The expressed assimilative capacity of each geochemical indicator at each monitoring point is calculated.
12. Select a contaminant and any one or two geochemical indicators to indicate consumption of the contaminant and production/consumption of geochemical indicators consistent with known biodegradation reactions (e.g., increased alkalinity, reduced dissolved oxygen concentrations in a source area well). The evaluation of geochemical indicators across a dissolved contaminant plume can be used in the demonstration of natural bioremediation. Any of the following trends (as shown in Table 4.5) observed across a contaminant plume (with higher contaminant concentrations) would suggest qualitatively that there is a strong potential for the occurrence of biodegradation:

Table 4.5. Expected Response of Geochemical Indicators

A relative Decrease in:	**A Relative Increase in:**
Dissolved Oxygen	***Ferrous Iron***
Nitrate	***Methane***
Sulfate	***Manganese***
Redox Potential	***Alkalinity***

13. The program provides a simultaneous plot of contaminants and geochemical indicators in a graph. This graphical presentation is also used for indicating existing anoxic and redox conditions along the overall ground water plume.

4.4 Module 4: Estimation of Contaminant Mass at a Source Zone

Source Zone Analysis:
See Figure B.4 of this User's Manual. This worksheet can be used to estimate a contaminant mass distribution at the source. At first, define the sampling area and three sampling zones (unsaturated, smear, saturated) associated with each sampling point using the Thiessen Polygon method. Collect and analyze samples to determine representative contaminant concentrations both laterally and vertically from the original release. Heterogeneous subsurface environments require more sampling layers to determine mass distribution. The method assumes that the concentration measured at a given point represents the concentration in the area out to a distance half-way to all adjacent sampling points. Refer to Appendix C of the guidance document

(Ecology Pub. No. 05-09-091) on how to assess/calculate the amount of contaminant source mass at a site.

1. Enter the logistical information: descriptive text for the identification of a particular site including site name, address, and any additional information.
2. Select a contaminant name from a drop-down menu to adjust the density of the pure chemical selected: the liquid density is used to convert the weight to a volume of contaminant.
3. Enter the measured thickness of each layer of sampling zones.
4. Enter the measured bulk density of each layer of sampling zones.
5. Enter the measured porosity and water content for the saturated zone layer only.
6. Enter the individual area and its associated concentration to represent a sample for each sampling zone. Each data point is correlated with an area represented by that data point. For the unsaturated zone, the worksheet can handle up to 40 data points. For smear and saturated zones, the worksheet can handle up to 24 data points.
7. The volume and weight of each soil layer of sampling zones is calculated. The weight of each soil layer in the sampling zones is calculated using the previously entered soil density.
8. The area-weighted average concentration is calculated for a given layer depth in each sampling zone.
9. The mass and volume of contaminant is calculated for a given layer depth in each sampling zone. Mass is calculated by multiplying average concentration and weight of each soil column layered. The volume of contaminant is calculated using the liquid density of pure contaminant assigned previously.
10. The relative mass distribution of contaminant among different source zones is calculated in terms of percent.

4.5 Input for Modules 5 and 6

When preliminary information obtained under Modules 1, 2, and 3 does not adequately demonstrate that natural attenuation is viable as a cleanup action, additional information may be necessary, and analytical modeling as explained in Modules 5 and 6 may be necessary. The objectives of Modules 5 and 6 are:

- To evaluate the contribution of biodegradation to the overall natural attenuation rate (for both Modules 5 and 6)
- To predict that the overall down-gradient plume is and will be stable, shrink, or expand over time (for Module 6 only)
- To estimate the restoration time to achieve a cleanup goal at a receptor location without further source removal (for Module 6 only)
- To estimate the additional amount of source to be removed in order to achieve a cleanup goal at a location under the specified restoration time frame (for Module 6 only)
- To estimate a contaminant mass loading rate to a nearby surface water body if any (for Module 6 only)

The log-linear regression and/or non-parametric analysis techniques described under Modules 1 and 2 yield attenuation information that does not distinguish among sorption, dispersion, and biodegradation. With given inputs, these evaluations above can be accomplished by using an analytical solution that includes advection, dispersion, sorption, and biodegradation for the stable (steady-state) and shrinking (transient-state) plumes. Modules 5 and 6 are based on the Domenico (1987; see footnote 9) analytical solute transport model. Domenico solution accounts for the effects of advective transport, 3-D dispersion, adsorption, and decay in the plume. In Module 6, for comparison purposes, the Domenico solution has been adapted to provide three different model types representing:

- Transport with "no biodegradation";
- Transport with "1st-order biodegradation"; and
- Transport with "instantaneous biodegradation reaction".

Note: The instantaneous biodegradation reaction model assumes that the actual mass leaving the source zone is equal to the sum of observed concentration and the expressed assimilative capacity. Very different source lifetimes may be obtained (and different results predicted) with the use of 1st-order biodegradation vs. instantaneous reaction models.

The analytical solution under 1-D for steady condition is used to estimate a site-specific biodegradation rate constant as explained under the Module 5. Module 5 relies on the assumptions that: the contaminant concentration is initially zero; a continuous contaminant concentration exists in the source; and, the transport is contained within a semi-infinite medium. The analytical solution under 2-D for transient condition is used to calibrate a site-specific biodegradation rate constant as explained under the Module 6.

Application of Modules 5 and 6 may be limited at some sites because ground water flow is greatly simplified, requiring assumptions of homogeneous aquifer properties and a steady ground water flow regime. This means that analytical solutions to the transport equation do not account for things such as heterogeneous aquifers, draw-down due to pumping wells, significant discharge to (or recharge from) surface water bodies, significant surface relief, more than one distinct contaminant source, or ground water flow divides. Furthermore, in these modules, advective transport of the contaminant is allowed to occur in only one dimension (plume center-line), and transport in other dimensions is due solely to dispersion.

Inputs for Transport Models (for Modules 5 and 6):
See Figure B.5.1 of this User's Manual. The input worksheet for Modules 5 and 6 is modified from BIOSCREEN (Newell et al., 1997[2]) Version 1.4 and is based on MS Excel® spreadsheet application of Domenico's (Domenico, 1987[9]) analytical solution of ground water flow. Refer to the original BIOSCREEN manual and US EPA's web-based interactive tool (On-Site: On-line Site Assessment Tool[10]) for a detailed explanation of input parameters and source dissolution terms if necessary.

When there is a high degree of uncertainty regarding the magnitude of inputs (or parameters) used in a model, the value of the parameters should be selected to err on the conservative side; i.e., tend to result in greater concentrations flowing at greater ground water velocities. Sensitivity analysis may be performed by varying parameters used in the model to identify key

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[9] Domenico, P.A., 1987, An Analytical Model for Multidimensional Transport of a Decaying contaminant Species, Journal of Hydrology, Vol. 91, pp 49-58.

[10] US EPA, 2003, Modeling subsurface Transport of Petroleum Hydrocarbons, http://www.epa.gov/athens/learn2model/part-two/onsite/index.html

input parameters having the greatest influence on predictions and to quantify the uncertainty in the calibrated model. It is recommended that the results of the sensitivity analysis be documented.

For completeness, additional scenarios can be modeled to bracket the upper and lower limits of any parameters, thereby demonstrating a range of likely plume extents for reasonable variations in input parameters. The model should be calibrated for the individual site. Hence, the value of biodegradation rate constant (λ, site-specific 1st-order biodegradation rate constant) that is considered as a key site-specific parameter is recommended to be calibrated with field data. Or, it can be normalized to a conservative tracer (e.g., chloride, trimethylbenzene, etc.) independently. It may not be appropriate to assume biodegradation rate constants or to use literature values for basic model inputs (such as hydraulic conductivity, contaminant mass in contaminant source) unless the Ecology site manager approves.

1. Before entering any data for this worksheet, carefully read the input instruction (located at the upper right corner of worksheet) applicable for only this worksheet. Note that a title marked with "*" is for Module 6 only. For example "*5. Source Release Time" is for the Module 6 calculation only. You do not need to provide these data for a Module 5 calculation. Click "symbols" underlined to see further US EPA web hyper-linked information.
2. Enter the logistical information: descriptive text for the identification of a particular site including site name, address, and any additional information.
3. Enter the seepage velocity directly or calculate this velocity with the model using data entered in the blue cells (hydraulic conductivity, hydraulic gradient, and effective porosity). If the calculation option does not appear to work, restore the formula by clicking on the "Restore Formula" button nearby.
4. Enter site-specific horizontal hydraulic conductivity. This parameter is a measure of an aquifer's ability to transmit ground water. The most common and reliable methods to estimate are slug/bail or pumping tests. Laboratory tests with standard ASTM or other methods described in hydrology textbooks could be used also. For conservative use, the high end of hydraulic conductivities measured at the site could be entered for the modeling. The formula to estimate seepage velocity used in the worksheet is as below:

$$v_{gw} = \frac{Ki}{n_e} \qquad \text{(Eq. 4.2)}$$

5. Enter a site-specific hydraulic gradient. This parameter is the slope of the water table for unconfined aquifers. A minimum of three wells (or piezometers) at a contaminated site drilled to the same depth into the geologic formation (in the same aquifer and intersecting the water table – not necessarily drilled to the same depth) is required to estimate the hydraulic gradient and ground water flow direction (x-direction). To determine ground water flow direction using only three wells, a trigonometric approach can be used ("three point problem"). Ground water flow direction also can be determined from water table data. In order to determine the effect of temporal and spatial variation in flow direction, quarterly water table measurements should be taken over at least one year. Refer to US EPA's web-based interactive tool (Gradient and Direction from Four or More Points:

http://www.epa.gov/athens/learn2model/part-two/onsite/gradient4plus-ns.htm) or Optimal Well Locator (US EPA, 2004[11]) for the calculation of hydraulic gradient and direction of ground water flow.

6. Enter a site-specific effective porosity. The effective porosity is the total porosity minus the specific retention, which is the amount of water that is retained in the medium against the force of gravity. A common method to estimate this parameter is a tracer test (e.g., bromide solution). One commonly used value for silts and sands is an effective porosity of 0.25. For conservative use, the low end of effective porosity measured/estimated at the site should be entered into the model.
7. Enter longitudinal dispersivity. Longitudinal dispersion is the process whereby a plume will spread out parallel to the direction of ground water flow due to mechanical mixing and chemical diffusion in the aquifer. Dispersion of a contaminant in a heterogeneous aquifer is a complex process and is caused mainly by ground water velocity variations at different scales. This variation is, in turn, affected by variations of hydraulic conductivity. Without detailed knowledge of these variations which is usually the case for most sites, accurate calculation of the dispersivity is difficult, and one has to rely on rough estimates. Ecology recommends selecting a value using a commonly used simple estimation technique (Xu and Eckstein, 1995[12] and Al-Suwaiyan, 1996[13]) based on the length, L_p (unit in feet) of the plume as below.

$$\alpha_x = 2.69 * \left[\log_{10}\left(\frac{L_p}{3.28} \right) \right]^{2.446} \qquad \text{(Eq. 4.3)}$$

   Refer to the User's Manual of BIOCHLOR (Aziz et al., 2000[14]) for more detailed discussion of longitudinal dispersivity estimates. Or, it can be adjusted to best-fit with field tracer data within the plume at a certain given time (calibration).
8. Enter transverse dispersivity. Transverse dispersion is the process whereby a plume will spread out perpendicular to the direction of ground water flow due to mechanical mixing and chemical diffusion in the aquifer. This value is commonly set to be equal to 10% of the longitudinal dispersivity value.

$$\alpha_y = 0.1\alpha_x \qquad \text{(Eq. 4.4)}$$

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[11] US EPA, 2004, Optimal Well Locator (OWL): A Screening Tool for Evaluating Locations of Monitoring Wells, EPA 600/C-04/017, Version 1.2, February 2004. http://www.epa.gov/ada/csmos/models/owl.html

[12] Xu, M. and Eckstein, Y., 1995, Use of Weighted Least-Squares Method in Evaluation of the Relationship Between Dispersivity and Field Scale, Ground water, 33(6):905-908.

[13] Al-Suwaiyan, M., 1996, Discussion of Weighted Least-Square Method in Evaluation of the Relationship Between Dispersivity and Field Scale. Discussion of Papers, Ground water, 34(4):578

[14] Aziz, C.E., Newell, C.J., Gonzales, J.R., Haas, P.E., Clement, T.P., and Sun, Y., 2000, BIOCHLOR: Natural Attenuation Decision Support System, User's Manual Version 1.0, pp.36-38, EPA/600/R-00/008, US EPA, Office of Research and Development, Washington D.C.

9. Enter vertical dispersivity. Vertical dispersion is the process whereby a plume will spread out vertically downward due to mechanical mixing and chemical diffusion in the aquifer. This value is commonly set to be equal to 2.5% of the longitudinal dispersivity value.

$$\alpha_z = 0.025\alpha_x \qquad \text{(Eq. 4.5)}$$

10. Enter the measured/estimated plume length (along the principal ground water flow direction) of the existing ground water plume. This value is often represented by the down-gradient distance between the source and the contour where the benzene concentration is 5 ug/L, which is the Method A ground water cleanup level.
11. Select or enter a contaminant name from the drop-down menu so that K_{oc} of the selected chemical can be selected from the database.
12. Enter the retardation factor of the selected ground water contaminant directly. Alternatively, it can be calculated with a formula using data entered in the blue cells (soil bulk density, partition coefficient, organic carbon fraction, effective porosity). This parameter describes the extent to which the migration of dissolved contaminants can be slowed by sorption to the aquifer matrix. The degree of retardation depends on both aquifer matrix and contaminant properties. If the calculation option does not appear to work, the formula (Eq. 4.6) can be restored by clicking on the "Restore Formula" button nearby.

$$R = 1 + \frac{K_{oc} f_{oc} \rho_b}{n_e} \qquad \text{(Eq. 4.6)}$$

13. Enter soil bulk density, which is the dry weight of the aquifer soil matrix divided by its total volume in an undisturbed state.
14. Enter the chemical-specific partition coefficient. Use K_{oc} values listed in the database provided unless the K_{oc} values are determined for the specific site using the procedures in WAC 173-340-747. In a case where a mixture of contaminants (e.g., BTEX) is simulated as a single contaminant, a value for the BTEX compounds can be assumed using values for the individual compounds weighted by their representative K_{oc}.
15. Enter organic carbon fraction. Samples for organic carbon should be taken from the same saturated horizon in which the contaminant transport occurs, but from an area that has not been impacted. To be conservative, the low end of the organic carbon fraction measured at the site should be entered into the model.
16. The velocity of the contaminant retarded by sorption (R) in the aquifer is calculated using the following equation (Eq. 4.7).

$$v_c = \frac{v_{gw}}{R} \qquad \text{(Eq. 4.7)}$$

17. The biodegradation rate constant (λ) is the parameter that describes the average rate at which a dissolved contaminant is being biodegraded based on an assumed 1st-order decay process. The amount of biodegradation that occurs is related to the time the contaminants spend in the

aquifer. This parameter is not related to the time it takes for the source concentration to decay at the source zone. In order to avoid significantly over-predicting or under-predicting actual biodegradation rates, considerable care should be exercised in the selection of this value for each contaminant. If known, enter a fixed biodegradation rate constant for the use of Module 6 (transient-state assumption).

Note: To calibrate the biodegradation rate constant under Module 6 or Module 5, it is necessary to enter an initial estimated value. A value of 1.0 yr^{-1} is a good initial value for petroleum-contaminated ground water that is relatively close to the final value and executes the optimization faster with consistent model results. Note that one "1" yr^{-1} will be the default that is an initial estimate for the optimization routine for further calibration against field data. Under Module 5, the biodegradation rate constant will be independently computed under steady-state assumption (Buscheck and Alcantar, 1995[15]). The calibrated λ will not be carried over to Module 5 but to Module 6.

18. The half-life of the selected contaminant is displayed on the basis of the biodegradation rate constant entered and/or calibrated in #17 against field data. This is the time that it takes the plume concentration to degrade by one-half as a contaminant migrates through the aquifer.

$$t_{1/2} = \ln(2)/\lambda = 0.693/\lambda \qquad \text{(Eq. 4.8)}$$

19. The calculated Chi-square statistics result for λ are displayed. See the detailed calibration procedure below (#27).
20. Enter the average background concentration minus the lowest observed concentration of each geochemical indicator for the specific use of instantaneous reaction model. These field data are also used for the calculation of maximum site-specific expressed assimilative capacity (using the utilization factors shown in the database) of ground water as it flows through the source zone and plume. These geochemical indicator data are not used to calibrate the site-specific λ for Module 6.
21. Site-specific total expressed assimilative capacity is displayed.
22. Enter the source release time, which is the period between the original releases (or the time a contaminant began moving in the ground water plume) and the date the field data were collected. This is used for Module 6 only.
23. For Module 6, enter source dimensions including the saturated source zone depth (or thickness), width, and its concentrations/soluble mass. Module 6 has simple source decay terms that can be used to evaluate source half-life based on ground water flow rate, source zone concentration, and source mass. Detail on the assumptions used to input source dimensions including the source dissolution formula for a declining source concentration can be found on pages of 27-32 of the User's Guide of BIOSCREEN (Newell et al., 1997[2]). For a constant concentration and continuous source, enter "infinite" for the entry cell of "soluble mass" to simulate the 2-D steady–state condition.

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[15] Buscheck, T.E. and Alcantar, C.M., 1995, Regression Techniques and Analytical Solutions to Demonstrate Intrinsic Bioremediation, in Proceeding of the 1995 Battelle International symposium on in-site and on-site, pp.109-116, Battelle Press.

24. Enter the name of monitoring well locations that will be used for the simulation. This input is optional for the identification of monitoring points. Leaving it blank will not affect calculation results.
25. The locations of the monitoring wells should be entered using a fixed two-dimensional coordinate system. Do **not** leave blank entries between data points. Enter the centerline distance (x-direction) measured between the monitoring point and the source zone as indicated on the worksheet for each monitoring point. Enter the perpendicular distance (y-direction) measured between the monitoring point and the plume centerline, as indicated on the worksheet for each monitoring point. Field data entered are used to help calibrate the biodegradation rate constant and are displayed with the predicted concentration in Modules 5 and 6.
26. Enter the representative concentration measured at each monitoring point after the release time specified previously in #22. Ecology recommends use of the median value of multiple measurements at each monitoring well. These data are used only to help calibrate the model (finding best-fitting value) and are displayed with model results. See Module 5 and the worksheet of "Comparison: Field data vs. Predicted" of Module 6.
27. The biodegradation rate constant can be calibrated by clicking on the "Calibration of Lambda" button for Module 6 only. The calibration method adopted to determine a site-specific "λ" involves finding a value that best matches the observed site-specific field contaminant concentration (that are normalized to the source concentration) from the entire site for a contaminant using non-linear regression techniques as applied to the 2-D Domenico analytical solution. The benefits of this chosen calibration method are:

    - It uses all of the available field contaminant data for the entire site so that it is not always required to place monitoring wells along the plume centerline;
    - It uses normalized concentrations as recommended by ASTM[16] (1995) to maximize the fit for overall plume data;
    - It integrates potential interactions among advection, sorption, dispersion, and biodegradation processes simultaneously; and
    - It is applicable to both steady (continuous source mode) and transient (finite source mode) source plumes.

    When the "Calibration" button is clicked, the "SOLVER" - an iterative spreadsheet routine function built in MS Excel® - is activated and attempts to minimize the difference between the user-supplied field contaminant data and the predicted data at overall sampling wells by varying the biodegradation rate constant. SOLVER tries different values for lambda until all the exit criteria set is met, as described in Figure 4.1. The Chi-Square statistic is used to test a goodness-of-fit for the non-linear regression technique herein. The closer to a value of one "1" of Chi-Square statistic, the better the goodness-of-fit.
28. All default formula can be restored to compute basic modeling input parameters such as seepage velocity, dispersivity, retardation, and half-life by clicking on the "Restore all Formulas…" button.

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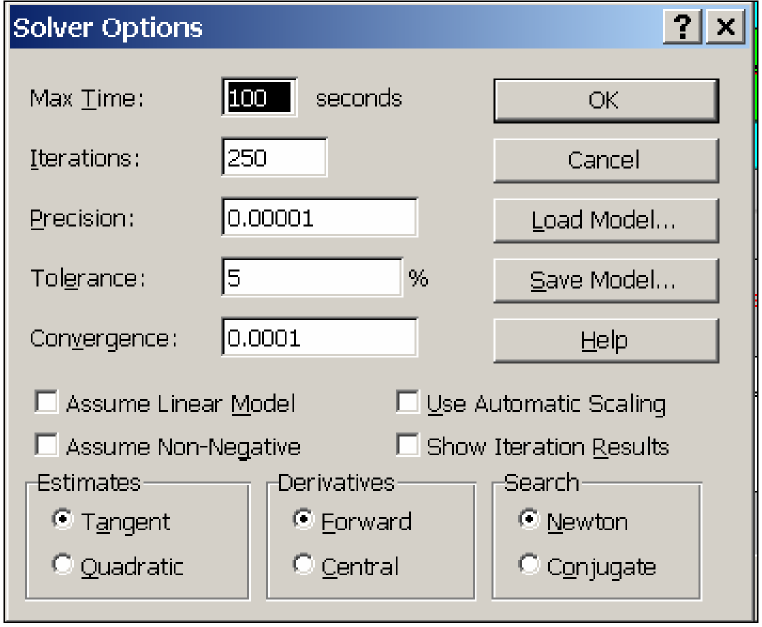
[16] ASTM, 1998, Standard Guide for Remediation of Ground water by natural attenuation at Petroleum Release Sites, pp 30-31, E1943-98.

Figure 4.1. Solver Options for “Calibration of Lambda”
(λ: site-specific biodegradation rate constant)



Max Time: 100 seconds
Iterations: 250
Precision: 0.00001
Tolerance: 5 %
Convergence: 0.0001

☐ Assume Linear Model
☐ Use Automatic Scaling
☐ Assume Non-Negative
☐ Show Iteration Results

Estimates
● Tangent
○ Quadratic

Derivatives
● Forward
○ Central

Search
● Newton
○ Conjugate

29. A set of example data can be pasted into the module by clicking on the “Paste Example Dataset” button.
30. This space is reserved for entering any additional descriptive site information if necessary.

4.6 Module 5: 1-D Steady-State Mode (Continuous Constant-Source)

In order to use Module 5, historical monitoring data collected for the entire plume should be used to determine if the plume is stable. In essence, this “steady-state” is achieved when any additional contamination released from the source is naturally attenuated at the same rate that it is introduced. As the source is depleted and the main loading rate of contaminants to ground water decreases, the plume begins to shrink.

It has been recently demonstrated that the method of Buscheck and Alcantar (1995: see footnote 15) usually overestimates the biodegradation rate constant by 21 - 65% for 2-D or 3-D plumes due to its usage of a solution to a 1-D advection-dispersion equation that does not consider lateral dispersion and finite source size. Refer to Zhang and Heathcote[17] (2003) for more detailed discussion. Thus, one should use extreme care when deriving the biodegradation rate constant developed under Module 5 with Buscheck and Alcantar. One of the conditions for using Buscheck and Alcantar’s steady-state model is that the selected down-gradient monitoring wells should be located along the plume centerline. In most sites, down-gradient monitoring wells may be off the plume centerline. In order to apply a 1-D model to these realistic cases, the distance between these off-centerline wells and source wells should somehow be converted to the centerline distance. In this analytical tool package, an ellipse trigonometric method is used to convert an off-centerline distance to a centerline distance. The ellipse shape is assumed based on

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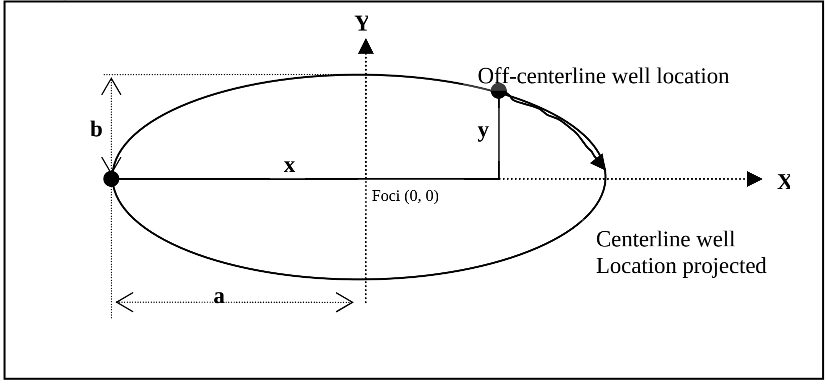
[17] Zhang, Y. and Heathcote, R.C., 2003, An Improved Method for Estimation of Biodegradation Rate with Field Data, Ground water Monitoring and Remediation, pp. 112-116, Vol. 23, No. 3.

observations that the plume migrates fastest along ground water flow direction, and the longitudinal dispersivity is greater than transverse dispersivity in general as demonstrated by Martin-Hayden and Robbins[18] (1997). The basic assumptions used in this conversion are:

- the ellipse width (major axis) = 33% of the ellipse length (minor axis) (ASTM, 1995[19]; US EPA, 1986[20]); and
- the ellipse is the contaminant iso-concentration line.

The equation for an ellipse with axis is written, and the shape of an ellipse can be drawn as shown in Figure 4.2:

Figure 4.2. Transformation of "off-centerline" well location



$$\frac{X^2}{a^2} + \frac{Y^2}{b^2} = 1 \qquad \text{(Eq. 4.9)}$$

Where,

a= the length of the major axis
b= the length of the minor axis: ***b = 0.33a***
X= the coordinate to the x dimension
Y= the coordinate to the y dimension
x = the distance in x-direction: ***X = x-a*** and ***x > a > b***
y = the off-centerline distance, y-direction: ***Y = y***

If the source well is assumed to be close to one end of the ellipse and a down-gradient well is assumed to be located on the ellipse line with an off-centerline distance "y", then a centerline distance "y" can be calculated as follows. The projected down-gradient centerline distance on the iso-concentration line is twice of "a". By substitution of equations below into the general ellipse equation (Eq. 4.10) above:

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[18] Martin-Hayden, J. M. and Robbins, G.A., 1997, Plume distortion and Apparent Attenuation Due to Concentration Averaging in Monitoring Wells., Ground water, pp 339-346, Vol. 35, No 2.

[19] American Society for Testing and Materials, 1995, Standard Guide for Risk-based Corrective Action Applied at Petroleum Release, ASTM E-1739-95, Philadelphia, PA.

[20] US EPA, 1986, Background document for the Ground-Water Screening Procedure to support 40 CFR Part 269: land disposal, EPA/530-SW-86-047.

$$\frac{(x-a)^2}{a^2}+\frac{y^2}{(0.33a)^2}=1 \qquad \text{(Eq. 4.10)}$$

Upon rearrangement, the length of major axis (or, the projected centerline distance) can be solved as:

The projected centerline distance = $2a = 2*\left(\frac{0.33^2x^2+y^2}{0.33^2*2x}\right)$ (Eq. 4.11)

Also, the following condition of 2-D well location should be met:

$$\frac{y}{x}\le 0.33 \qquad \text{(Eq. 4.12)}$$

<u>Calculation of Rate Constants (1-D Steady State Mode): Temporal/Spatial Prediction:</u> See Figure B.5.2 of this User's Manual.

1. Logistical information is carried over from the worksheet of "Inputs for Transport Models".
2. All input parameters including current source concentration being used for steady state/continuous source mode simulation are displayed.
3. Enter the level of confidence to be used to estimate the boundary value of slope (calculated with log-linear regression analysis) and all consequent calculation results. Ecology recommends using a default confidence level of 85% or higher to better define the uncertainty involved in estimating the bulk attenuation rate and biodegradation rate constants.
4. The field data entered previously in the worksheet "Inputs for Transport Models" is plotted against the projected centerline distance from the source and field measured concentrations, and its log-linear regression result is displayed.
5. Average and lower boundary slopes of the log-linear regression line (concentration vs. centerline distance), coefficient of determination (r^2), and correlation coefficient (*r*) are calculated for given ground water contaminant data collected for the overall plume. The variable "*r*" measures the strength of a linear relationship between the centerline distance and log concentration of the contaminant. The number (*n*) of ground water contaminant data used for a log-linear regression is also displayed. As explained previously for Module 2, "*r*" and "*n*" are used to calculate the confidence level that is used to determine whether there is adequate evidence to conclude that there is a significant linear correlation between sampling distance and log contaminant concentration for the overall plume.
6. The Student's t-statistic is calculated using the Pearson correlation coefficient, and the corresponding level of confidence is calculated to determine whether there is sufficient evidence to conclude that there is a significant linear correlation between sampling distance and log contaminant concentration.
7. The average and lower boundary (@ a predetermined level of confidence) bulk attenuation rate and biodegradation rate constants are calculated and displayed. The regression of contaminant concentration vs. centerline distance produces the bulk attenuation rate constant (k) using the following equation:

$$C_x = C_{start} * \exp\left(-k\frac{x}{v_c}\right) \qquad \text{(Eq. 4.13)}$$

The equation that produces the biodegradation rate constant (λ) under 1-D is based on Buscheck and Alcantar's 1-D steady-state formula (on page 31 see footnote 15) shown as below.

$$\lambda = \frac{v_c}{4\alpha_x} * \left\{\left[1 + 2\alpha_x\left(\frac{k}{v_{gw}}\right)\right]^2 - 1\right\} \qquad \text{(Eq. 4.14)}$$

8. The ratio (λ/k) of the contribution of biodegradation to the overall bulk attenuation rate (expressed as %), is displayed.
9. Enter the locations (distance in x and y-directions) of the down-gradient receptor to predict the concentration. Enter the simulation time at the receptor's location.
10. The average and lower boundary concentrations predicted are displayed at the receptor's location, and simulation time is entered. As shown below, Bear's 1-D model (1979[21]) with first-order decay and constant concentration and continuous source model (Eq. 4.15) is used to predict the concentration as a function of time and distance in x-direction.

$$C_{x,t} = \left(\frac{C_o}{2}\right) * \exp\left\{\left(\frac{x}{2\alpha_x}\right) * \left[1 - \sqrt{\left(1 + \frac{4\lambda\alpha_x}{v_c}\right)}\right]\right\} * erfc\left\{\frac{\left[x - v_c t\sqrt{\left(1 + \frac{4\lambda\alpha_x}{v_c}\right)}\right]}{2\sqrt{\alpha_x v_c t}}\right\} \qquad \text{(Eq. 4.15)}$$

11. Enter the target ground water cleanup level at the receptor's location. This enables estimation of the target source concentration for the condition specified in #9.
12. The target concentration of source needed to achieve the target ground water concentration at the given receptor location is calculated with the Bear model (1979) and displayed by pressing the "Calculate Target Source Concentration" button. This computation is conducted with the average slope calculated by the log-linear regression technique and the average seepage velocity given.
13. Temporal and spatial predictions using the Bear Model (1979) as a function of projected centerline distance (@ a receptor's given location) and time (@ a simulation time given previously) are displayed. This computation is conducted with both the average and lower boundary slopes (@ a predetermined confidence level) calculated by the log-linear regression technique and the seepage velocity given.

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[21] Bear, J., 1979, Hydraulics of Ground water, pp. 268-269, McGraw Hill, New York.

4.7 Module 6: 2-D Transient-State Mode (with Decaying-source)

As described previously, Module 6 is based on the Domenico (1987[9]) analytical solute transport model. For comparison purposes, the 3-D Domenico solution has been adapted to provide three different types representing:

- Transport with "no biodegradation" with the following equation (Eq. 4.16):

$$C_{x,y,z,t} = \frac{1}{8}C_o * \exp\left[-k_{source}\left(t - \frac{x}{v_c}\right)\right] * erfc\left\{\frac{\left[x - v_c t\right]}{2\sqrt{\alpha_x v_c t}}\right\} *$$

$$\left\{erf\left[\frac{\left(y + \frac{Y}{2}\right)}{2\sqrt{\alpha_y x}}\right] - erf\left[\frac{\left(y - \frac{Y}{2}\right)}{2\sqrt{\alpha_y x}}\right]\right\} * \left\{erf\left[\frac{\left(z + \frac{Z}{2}\right)}{2\sqrt{\alpha_z x}}\right] - erf\left[\frac{\left(z - \frac{Z}{2}\right)}{2\sqrt{\alpha_z x}}\right]\right\} \quad \text{(Eq. 4.16)}$$

- Transport with "1st-order biodegradation" with the following equation (Eq. 4.17):

$$C_{x,y,z,t} = \frac{1}{8}C_o * \exp\left[-k_{source}\left(t - \frac{x}{v_c}\right)\right] * \exp\left\{\left(\frac{x}{2\alpha_x}\right)\left[1 - \sqrt{\left(1 + \frac{4\lambda\alpha_x}{v_c}\right)}\right]\right\} * erfc\left\{\frac{\left[x - v_c t\sqrt{\left(1 + \frac{4\lambda\alpha_x}{v_c}\right)}\right]}{2\sqrt{\alpha_x v_c t}}\right\} * \quad \text{(Eq. 4.17)}$$

$$\left\{erf\left[\frac{\left(y + \frac{Y}{2}\right)}{2\sqrt{\alpha_y x}}\right] - erf\left[\frac{\left(y - \frac{Y}{2}\right)}{2\sqrt{\alpha_y x}}\right]\right\} * \left\{erf\left[\frac{\left(z + \frac{Z}{2}\right)}{2\sqrt{\alpha_z x}}\right] - erf\left[\frac{\left(z - \frac{Z}{2}\right)}{2\sqrt{\alpha_z x}}\right]\right\}$$

- Transport with "instantaneous biodegradation reaction" with the following equation (Eq. 4.18):

$$C_{x,y,z,t} = \frac{1}{8}C_o * \exp\left[-k_{source}\left(t - \frac{x}{v_c}\right) - AC\right] * erfc\left\{\frac{\left[x - v_c t\right]}{2\sqrt{\alpha_x v_c t}}\right\} *$$

$$\left\{erf\left[\frac{\left(y + \frac{Y}{2}\right)}{2\sqrt{\alpha_y x}}\right] - erf\left[\frac{\left(y - \frac{Y}{2}\right)}{2\sqrt{\alpha_y x}}\right]\right\} * \left\{erf\left[\frac{\left(z + \frac{Z}{2}\right)}{2\sqrt{\alpha_z x}}\right] - erf\left[\frac{\left(z - \frac{Z}{2}\right)}{2\sqrt{\alpha_z x}}\right]\right\} - AC \quad \text{(Eq. 4.18)}$$

Comparison: Field Data vs. Predicted by Three Models:
See Figure B.6.1 of this User's Manual.

1. Logistical information is carried over from the worksheet titled, "Inputs for Transport Models".

2. The simulation time (or the release time entered previously in the input worksheet) associated with the predicted well concentration is displayed.
3. The name and location of each monitoring point used for the simulation are displayed.
4. The output displays predicted concentrations (as well as normalized concentrations) in a tabular form along the monitoring wells with respect to three different types of models against field-measured concentrations at each monitoring point. The predicted concentration is the average concentration at the top of the saturated zone (assuming that $z = 0$) on the basis of 2-D location of the monitoring point and release time.
5. The predicted concentrations (as well as normalized concentrations) for the monitoring wells with respect to three different types of models against field-measured concentrations at each monitoring point are plotted for a visual comparison.

<u>Calculation of Mass Removal Rate by Biodegradation:</u>
See Figure B.6.2 (a, b, c, d) of this User's Manual.

1. Opening worksheet: Logistical information is carried over from the worksheet of "Inputs for Transport Models". See Figure B.6.2.a of this User's Manual.
2. One of three different models can be selected by pressing one of three buttons displayed on the worksheet. See Figure B.6.2.b of this User's Manual.
3. The predicted down-gradient concentration calculated by the selected model is displayed as tabulated numerical results.

- See Figure B.6.2.b of this User's Manual for "1st-order Decay Model."
- See Figure B.6.2.c of this User's Manual for "No-biodegradation Model."
- See Figure B.6.2.d of this User's Manual for "Instantaneous Model."

4. Enter the lowest ground water concentration to display the plume's predicted output.
5. The 3-D graphic array shows the model prediction selected on the specified "10 x 5" grid. To alter the modeled area, fine-tune the model area width and length parameters on the worksheet. Enter the physical dimensions of the rectangular area to be modeled. Values should be appropriate to catch enough plume contaminant mass and small enough to show the whole 3-D graphic array.
6. Enter the simulation time to predict down-gradient concentrations. See Figure B.6.2.b of this User's Manual for different simulation times. Note that the name of the model associated with the predicted concentration is shown.
7. All data can be displayed or plotted by pressing the "Plot All data" button. Or, only data that exceeds the target ground water concentration entered above can be displayed or plotted by pressing the "Plot Data>Target" button.
8. The total amount of dissolved contaminant mass that has left the source zone. If the source is an infinite source, then the calculation is based on the discharge of ground water through the source zone (ground water seepage velocity times the total source width times the source depth) times the average concentration of the source zone (a weighted average of concentration and source length for each of the different source zones) times the simulation time. If the source is a declining source, an exponential decay term is used to estimate the mass of contaminant that has left source zone. The source decay term is for dissolution of soluble contaminant from the source zone.

9. The total amount of dissolved contaminant mass at the time when the field data are collected (after the release time) is calculated by integrating the mass of contaminant distributed all over the plume.
10. The amount and percent of dissolved contaminant that was removed/degraded in the plume due to biodegradation is provided.
11. The amount of each geochemical indicator that is consumed/produced by biodegradation is displayed. These values will appear under the selection of Instantaneous Model only.
12. The initial soluble mass in NAPL and soil source at the time of release (that was entered previously by the user) is displayed again to show the mass balance calculation.
13. The amount of mass remaining in the source zone at the simulation time specified is displayed. Actual value displayed will be different depending upon the choice of model type.
14. The volume of the ground water plume that exceeds the target ground water concentration (entered previously) is displayed.
15. The rate of ground water flow through the source zone dimension (source width, depth, seepage velocity, porosity) as defined previously by the user is displayed.

Note: When any output box display "Can't Calc", simply readjust (usually, increase) the modeled area length and width to barely capture most of the contaminant mass in the plume.

<u>Calculation of Target Source Mass and Restoration Time:</u>
See Figure B.6.3 of this User's Manual. This worksheet should be able to calculate the concentration profile of contaminant species at any monitoring point down-gradient of a ground water plume and any future simulation time.

1. Logistical information is carried over from the worksheet entitled "Inputs for Transport Models".
2. Input parameters being used for the simulation under the transient-state/decaying source mode are displayed.
3. Enter the starting and ending simulation time of contaminant migration at a specified down-gradient receptor location.
4. Enter the target ground water level to be cleaned up at the specified receptor's location.
5. Enter the location (distance in x and y-directions) of the specified down-gradient receptor.
6. Predictive plots of concentration vs. time at two different receptor locations are displayed with respect to two different types of models: No Degradation Model and 1st-order decay model.
7. The approximate/theoretical time required to reach one-half the steady-state concentration (or maximum concentration) at a given receptor location is displayed. This information can be used to check on how long it takes to reach a steady-state (or maximum concentration) condition. The formula (ASTM, 1998, see footnote 16) used to calculate the time required to reach one-half the steady-state concentration at a point along the x-direction of the plume is:

$$t = \frac{Rx}{V_{gw} * \sqrt{1 + \frac{4\alpha_x \lambda R}{V_{gw}}}} \qquad \text{(Eq. 4.19)}$$

8. Predicted concentrations (with respect to the type of model selected) at a given location and simulation ending time (and ½ of ending time) are displayed.
9. The restoration time to reach a target level at a given receptor location is computed and displayed by pressing the "Calculate Restoration Time" button. This computation is conducted under the current conditions (input parameters shown on the top left corner of this worksheet). Whenever the input parameters are changed from the worksheet of "Inputs for Transport Model", re-click this button to generate new information on restoration time. This is a backward calculation.

   Note: When "infinite" is entered for the entry cell of "soluble mass" (refer to #23 of "Inputs for Transport Models"), this "Calculate Restoration Time" button will not work properly.

10. The estimated amount of source mass needing to be removed to reach the target ground water concentration at a given receptor location and simulation ending time is calculated and displayed by pressing the "Calculate Target Source Mass" button. Whenever the input parameters are changed, re-click this button to generate new information on source mass.
11. Enter the assumed plume centerline distance and simulation time under the transient-state/decaying source mode to predict the temporal/spatial distribution of contaminants. The 1st-order decay model is used for this simulation.
12. Predictive plots of concentration and its temporal variation (for the specified simulation time) over the plume centerline distance are displayed with respect to the 1st-order decay model.

Calculation of Surface Water Mass Loading Rate:
See Figure B.6.4 of this User's Manual. This worksheet can be used to estimate the average ground water concentration in a vertical cross-section of the ground water plume and mass loading rate of the ground water plume into the nearby surface water body. Domenico's 3-D analytical solution with 1st-order biodegradation model is used for this simulation

1. Logistical information is carried over from the worksheet of "Inputs for Transport Models".
2. Enter the simulation time of contaminant release at a down-gradient surface water body nearby.
3. Enter the centerline distance (x-direction) from the source to surface water body.
4. Enter appropriate modeled area plume width and depth in order to catch enough plume contaminant mass flux.
5. Concentrations predicted as a function of simulation time, distance, plume depth, and width are displayed in tabular form.
6. A 3-D plot of concentration vs. depth and width of plume at given location of surface water body is displayed.
7. Vertical dispersivity used for prediction is displayed. Default: $\alpha_z = 0.025 * \alpha_x$.
8. The highest plume concentration in a vertical cross-section of ground water plume entering the surface water body at the simulation time is displayed. The rate of plume flow is displayed.
9. The average plume concentration in a vertical cross-section of ground water plume and the mass loading rate of contaminant through the cross-section of the plume into the surface water body is displayed.

Modification from BIOSCREEN Version 1.4:

The formula for the 3-D Domenico analytical solute transport model used in BIOSCREEN 1.4 (see page 39 of this User's Manual) are exactly the same as those used in Inputs worksheet and Module 6 of the Data Analysis Tool Package B. However, the following modifications were made in order to enhance the ability of the model to assess the effectiveness of natural attenuation.

- Features (functions or buttons) deleted from BIOSCREEN:
  - Two buttons "Calculate Animation" and "Recalculate this Sheet" and associated codes were deleted from the worksheet of "Centerline Output" of BIOSCREEN 1.4.

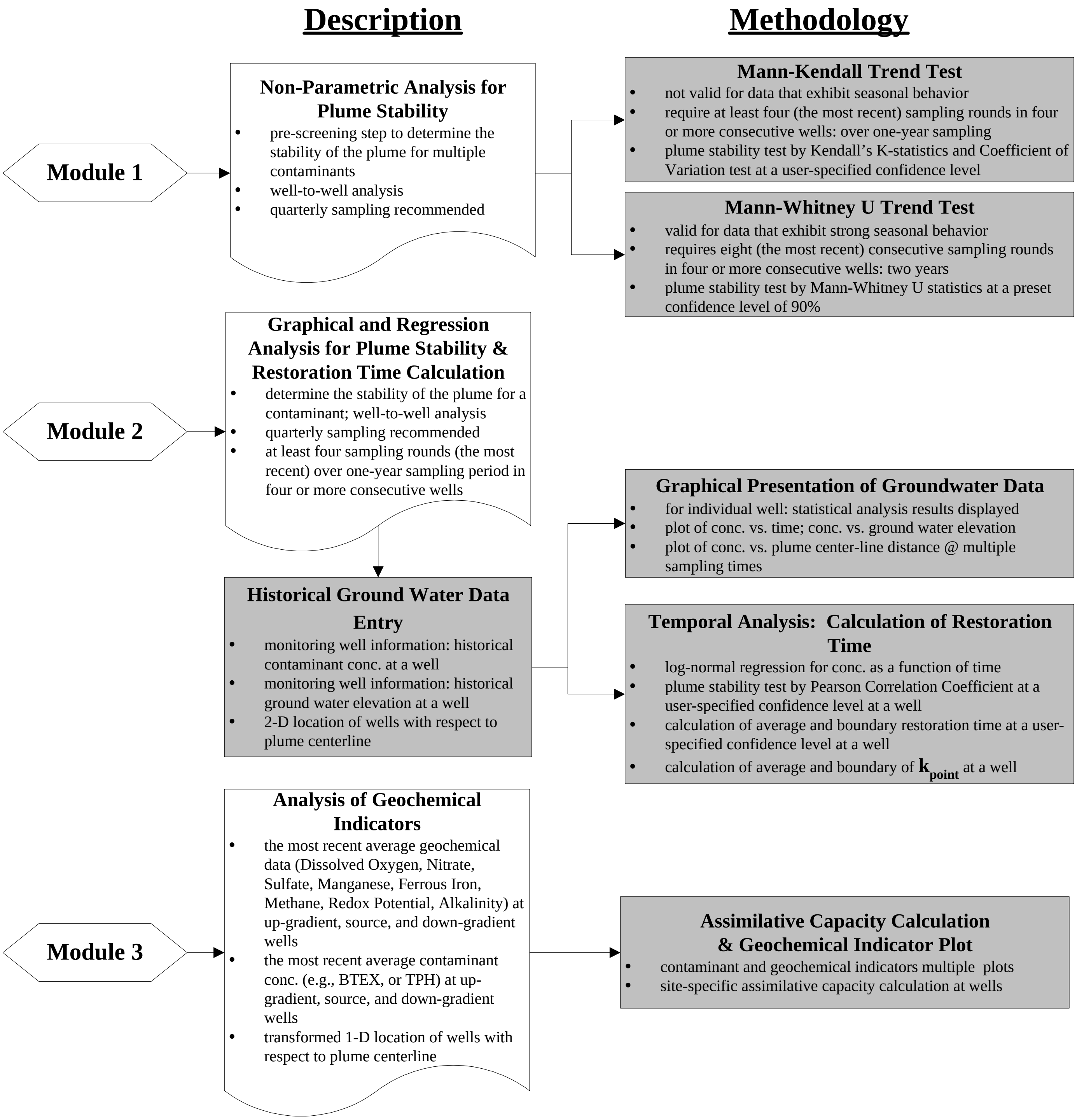
- Features (functions, buttons, worksheets) added/modified:
  - "Input for Transport Models" worksheet:
    - ✓ US EPA web base for further information is hyper-linked at the underlined symbols.
    - ✓ Symbols, abbreviations, and units have been changed in accordance with Appendix F of this guidance document (Pub. No. 05-09-091A)
    - ✓ A worksheet table of properties (e.g., utilization factors, solubilities, molecular weight, etc.) of contaminants commonly found at petroleum-contaminated sites is added.
    - ✓ An entry cell for Manganese to calculate the expressed assimilative capacity is added.
    - ✓ A separate button for "Restore Formula" is added for hydrogeology, dispersion, and adsorption terms, respectively.
    - ✓ The formula to estimate the site-specific longitudinal dispersivity has been changed to reflect the most recent findings.
    - ✓ 1st-order biodegradation rate constant: this constant is being calibrated by Chi-square statistics instead of visually fitting by trial-and-error, which is very subjective. This calibration can be made by pressing "Calibration of Lambda" button.
    - ✓ Field data for comparison (or calibration): the format for well information has changed from 1-D to 2-D so that all available wells concentrations can be used instead of wells located only in the plume centerline. Wells can be located anywhere in the plume unlike BIOSCREEN.
    - ✓ The modeled area (length and width) description was moved to the "Calculation of Mass Removal Rate by Biodegradation" worksheet.
    - ✓ Blank space is provided for a site description.
  - "Comparison: Field Data vs. Predicted by three models" worksheet:
    - ✓ Information has been added in graphical and tabular form showing the "normalized ground water concentration along the plume centerline".
    - ✓ A line has been added to show 2-D location (distance from the source, x, y-direction).
  - "Calculation of Mass Removal Rate by Biodegradation" worksheet:
    - ✓ The data entry for simulation time is added to simulate the contaminant concentration distribution as a function of time.
  - Two new worksheets have been added:
    - ✓ "Calculation of Target Source Mass and Restoration Time" worksheet has been added to predict temporal/spatial distribution of contaminant and to calculate the restoration time.
    - ✓ "Surface Water Loading Rate" worksheet has been added to calculate the mass loading rate to a nearby surface water body.

Appendix A

Calculation Modules for Evaluation of Natural Attenuation

Figure A.1. Calculation Module for Natural Attenuation Analysis
Package A

Note: Modules are not linked each other.



Non-Parametric Analysis for Plume Stability

- pre-screening step to determine the stability of the plume for multiple contaminants
- well-to-well analysis
- quarterly sampling recommended

Mann-Kendall Trend Test

- not valid for data that exhibit seasonal behavior
- require at least four (the most recent) sampling rounds in four or more consecutive wells: over one-year sampling
- plume stability test by Kendall's K-statistics and Coefficient of Variation test at a user-specified confidence level

Mann-Whitney U Trend Test

- valid for data that exhibit strong seasonal behavior
- requires eight (the most recent) consecutive sampling rounds in four or more consecutive wells: two years
- plume stability test by Mann-Whitney U statistics at a preset confidence level of 90%

Graphical and Regression Analysis for Plume Stability & Restoration Time Calculation

- determine the stability of the plume for a contaminant; well-to-well analysis
- quarterly sampling recommended
- at least four sampling rounds (the most recent) over one-year sampling period in four or more consecutive wells

Historical Ground Water Data Entry

- monitoring well information: historical contaminant conc. at a well
- monitoring well information: historical ground water elevation at a well
- 2-D location of wells with respect to plume centerline

Graphical Presentation of Groundwater Data

- for individual well: statistical analysis results displayed
- plot of conc. vs. time; conc. vs. ground water elevation
- plot of conc. vs. plume center-line distance @ multiple sampling times

Temporal Analysis: Calculation of Restoration Time

- log-normal regression for conc. as a function of time
- plume stability test by Pearson Correlation Coefficient at a user-specified confidence level at a well
- calculation of average and boundary restoration time at a user-specified confidence level at a well
- calculation of average and boundary of $\mathbf{k}_{\mathbf{point}}$ at a well

Analysis of Geochemical Indicators

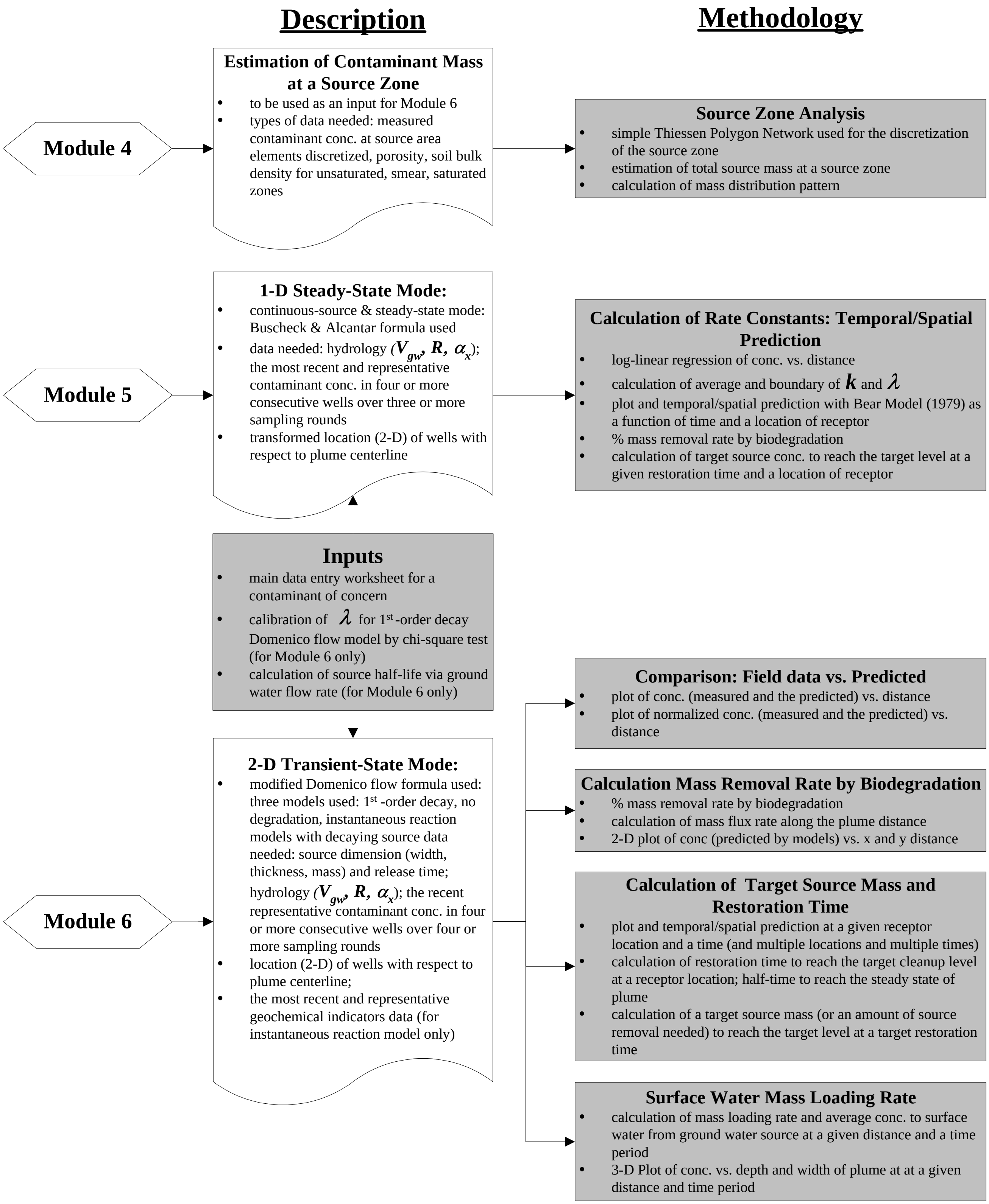
- the most recent average geochemical data (Dissolved Oxygen, Nitrate, Sulfate, Manganese, Ferrous Iron, Methane, Redox Potential, Alkalinity) at up-gradient, source, and down-gradient wells
- the most recent average contaminant conc. (e.g., BTEX, or TPH) at up-gradient, source, and down-gradient wells
- transformed 1-D location of wells with respect to plume centerline

Assimilative Capacity Calculation & Geochemical Indicator Plot

- contaminant and geochemical indicators multiple plots
- site-specific assimilative capacity calculation at wells

Figure A.2. Calculation Module for Natural Attenuation Analysis Package B

Note: Modules 5 and 6 share the same input worksheet.



Description

Methodology

Module 4

Estimation of Contaminant Mass at a Source Zone
- to be used as an input for Module 6
- types of data needed: measured contaminant conc. at source area elements discretized, porosity, soil bulk density for unsaturated, smear, saturated zones

Source Zone Analysis
- simple Thiessen Polygon Network used for the discretization of the source zone
- estimation of total source mass at a source zone
- calculation of mass distribution pattern

Module 5

1-D Steady-State Mode:
- continuous-source & steady-state mode: Buscheck & Alcantar formula used
- data needed: hydrology (V_{gw}, R, α_x); the most recent and representative contaminant conc. in four or more consecutive wells over three or more sampling rounds
- transformed location (2-D) of wells with respect to plume centerline

Calculation of Rate Constants: Temporal/Spatial Prediction
- log-linear regression of conc. vs. distance
- calculation of average and boundary of k and λ
- plot and temporal/spatial prediction with Bear Model (1979) as a function of time and a location of receptor
- % mass removal rate by biodegradation
- calculation of target source conc. to reach the target level at a given restoration time and a location of receptor

Inputs
- main data entry worksheet for a contaminant of concern
- calibration of λ for 1st -order decay Domenico flow model by chi-square test (for Module 6 only)
- calculation of source half-life via ground water flow rate (for Module 6 only)

Module 6

2-D Transient-State Mode:
- modified Domenico flow formula used: three models used: 1st -order decay, no degradation, instantaneous reaction models with decaying source data needed: source dimension (width, thickness, mass) and release time; hydrology (V_{gw}, R, α_x); the recent representative contaminant conc. in four or more consecutive wells over four or more sampling rounds
- location (2-D) of wells with respect to plume centerline;
- the most recent and representative geochemical indicators data (for instantaneous reaction model only)

Comparison: Field data vs. Predicted
- plot of conc. (measured and the predicted) vs. distance
- plot of normalized conc. (measured and the predicted) vs. distance

Calculation Mass Removal Rate by Biodegradation
- % mass removal rate by biodegradation
- calculation of mass flux rate along the plume distance
- 2-D plot of conc (predicted by models) vs. x and y distance

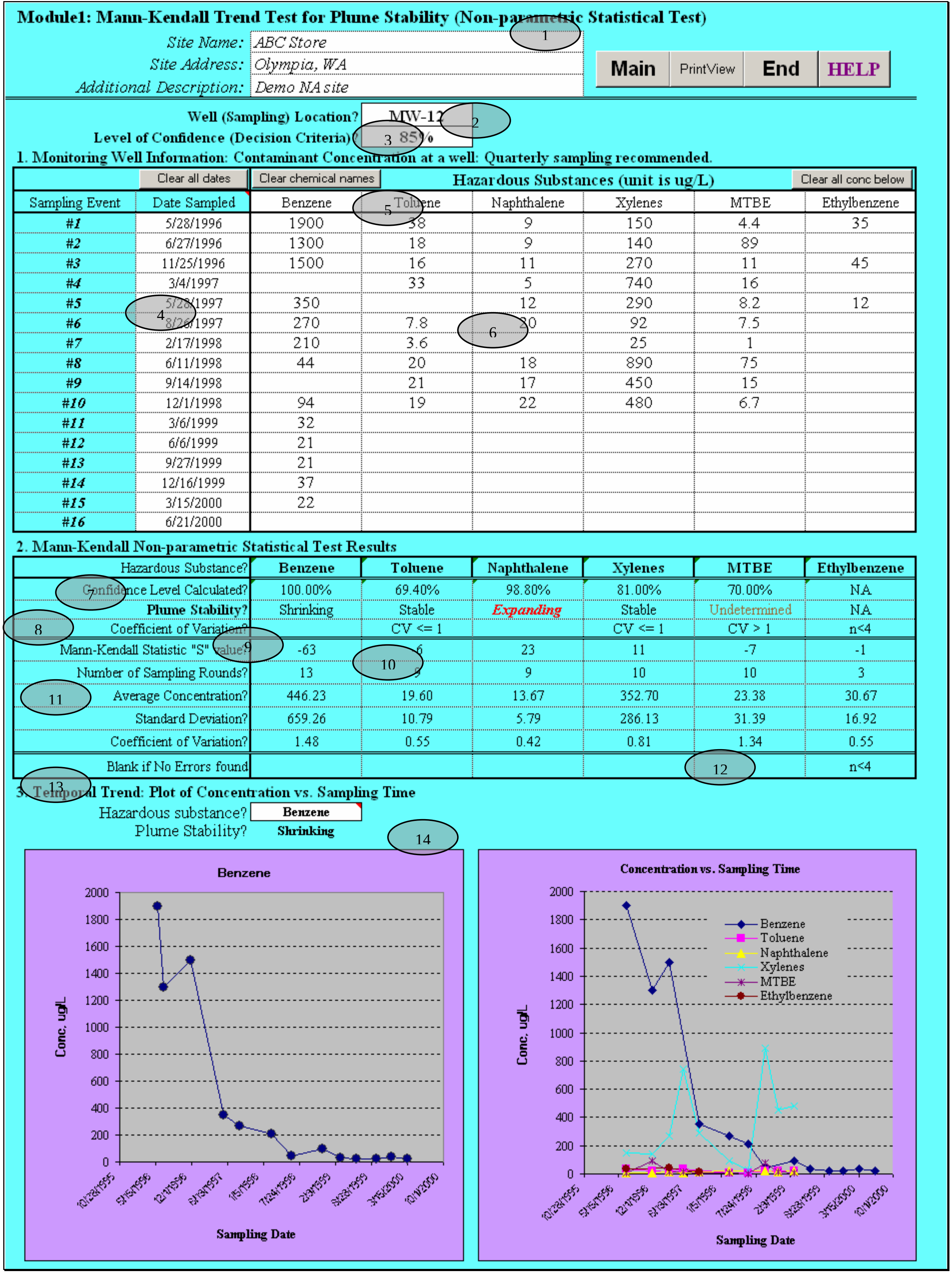
Calculation of Target Source Mass and Restoration Time
- plot and temporal/spatial prediction at a given receptor location and a time (and multiple locations and multiple times)
- calculation of restoration time to reach the target cleanup level at a receptor location; half-time to reach the steady state of plume
- calculation of a target source mass (or an amount of source removal needed) to reach the target level at a target restoration time

Surface Water Mass Loading Rate
- calculation of mass loading rate and average conc. to surface water from ground water source at a given distance and a time period
- 3-D Plot of conc. vs. depth and width of plume at at a given distance and time period

Appendix B

Calculation Worksheets

Figure B.1.1. Mann-Kendall Trend Test for Plume Stability (Non-parametric Statistical Test)



Module1: Mann-Kendall Trend Test for Plume Stability (Non-parametric Statistical Test)

Site Name:	*ABC Store*
Site Address:	*Olympia, WA*
Additional Description:	*Demo NA site*

Well (Sampling) Location? MW-12

Level of Confidence (Decision Criteria)? 85%

1. Monitoring Well Information: Contaminant Concentration at a well: Quarterly sampling recommended.

Hazardous Substances (unit is ug/L)

Sampling Event	Date Sampled	Benzene	Toluene	Naphthalene	Xylenes	MTBE	Ethylbenzene
#1	5/28/1996	1900	38	9	150	4.4	35
#2	6/27/1996	1300	18	9	140	89	
#3	11/25/1996	1500	16	11	270	11	45
#4	3/4/1997		33	5	740	16	
#5	5/28/1997	350		12	290	8.2	12
#6	8/26/1997	270	7.8	20	92	7.5	
#7	2/17/1998	210	3.6		25	1	
#8	6/11/1998	44	20	18	890	75	
#9	9/14/1998		21	17	450	15	
#10	12/1/1998	94	19	22	480	6.7	
#11	3/6/1999	32					
#12	6/6/1999	21					
#13	9/27/1999	21					
#14	12/16/1999	37					
#15	3/15/2000	22					
#16	6/21/2000						

2. Mann-Kendall Non-parametric Statistical Test Results

Hazardous Substance?	**Benzene**	**Toluene**	**Naphthalene**	**Xylenes**	**MTBE**	**Ethylbenzene**
Confidence Level Calculated?	100.00%	69.40%	98.80%	81.00%	70.00%	NA
Plume Stability?	Shrinking	Stable	***Expanding***	Stable	Undetermined	NA
Coefficient of Variation?		CV <= 1		CV <= 1	CV > 1	n<4
Mann-Kendall Statistic "S" value?	-63	6	23	11	-7	-1
Number of Sampling Rounds?	13	9	9	10	10	3
Average Concentration?	446.23	19.60	13.67	352.70	23.38	30.67
Standard Deviation?	659.26	10.79	5.79	286.13	31.39	16.92
Coefficient of Variation?	1.48	0.55	0.42	0.81	1.34	0.55
Blank if No Errors found						n<4

3. Temporal Trend: Plot of Concentration vs. Sampling Time

Hazardous substance? **Benzene**

Plume Stability? **Shrinking**

Figure B.1.2. Upper-Tail Probabilities for the Null distribution of Kendall’s S Statistics

Module 1: Upper-Tail Probabilities for the Null Distribution of Kendall's "S" Statistics

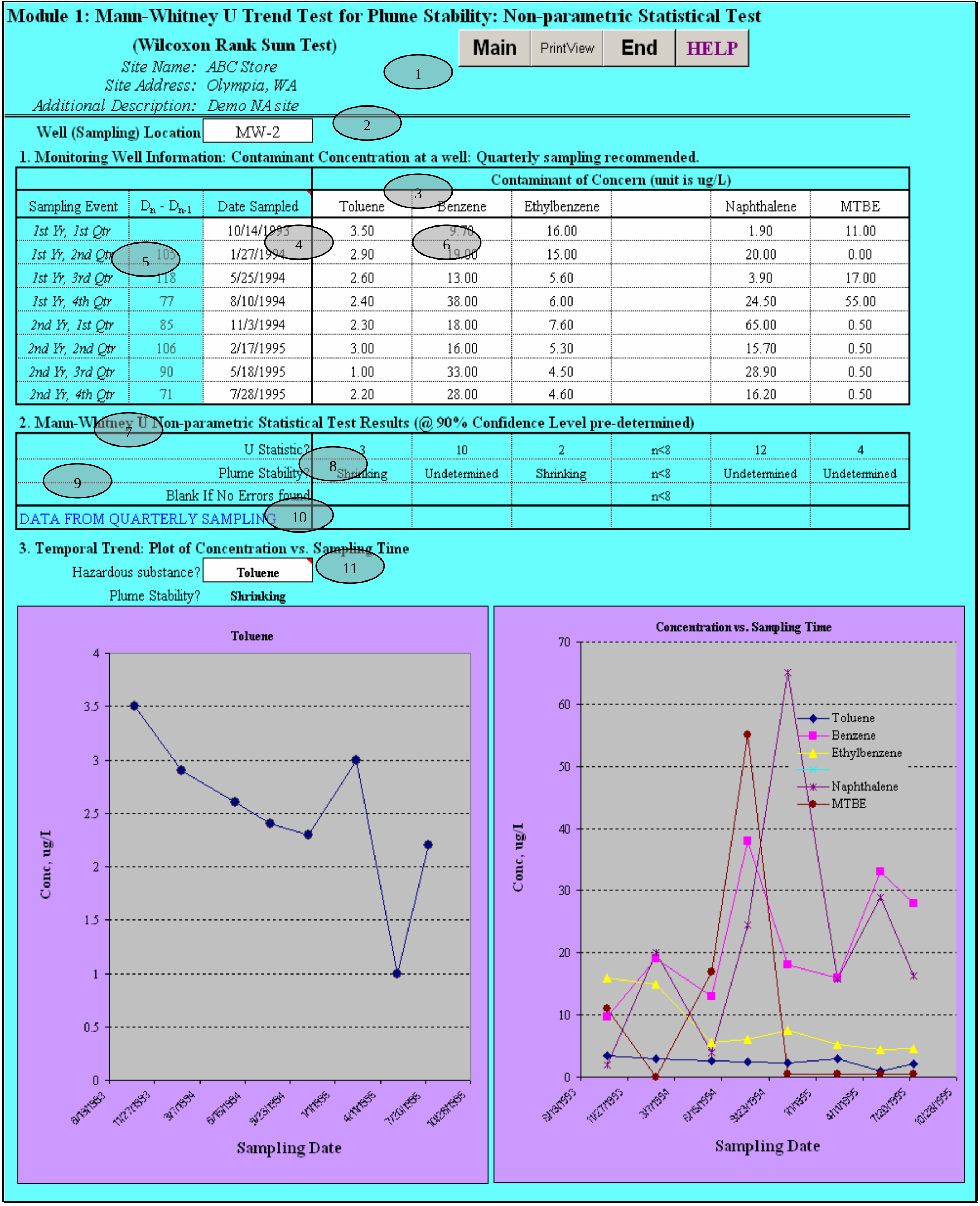
Adapted from
*Gilbert, R.O., "Statistical Methods for Environmental Pollution Monitoring, Van Nostrand Reinhold, 1987, Table A18.
*Hollander, M. and Wolfe, D.A., "Nonparametric Statistical Methods, Wiley, New York, 1973, Table A.21.

"S"	Number of Sampling Rounds														
Value	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**20**
0	0.625	0.592			0.548	0.540			0.527	0.524			0.518	0.516	0.513
1			0.500	0.500			0.500	0.500			0.500	0.500			
2	0.375	0.408			0.452	0.460			0.473	0.476			0.482	0.484	0.487
3			0.360	0.386			0.431	0.440			0.457	0.461			
4	0.167	0.242			0.360	0.381			0.420	0.429			0.447	0.452	0.462
5			0.235	0.281			0.364	0.381			0.415	0.423			
6	0.042	0.117			0.274	0.306			0.369	0.383			0.412	0.420	0.436
7			0.136	0.191			0.300	0.324			0.374	0.385			
8		0.042			0.199	0.238			0.319	0.338			0.378	0.388	0.411
9			0.068	0.119			0.242	0.271			0.334	0.349			
10		0.008			0.138	0.179			0.273	0.295			0.345	0.358	0.387
11			0.028	0.068			0.190	0.223			0.295	0.313			
12					0.089	0.130			0.230	0.255			0.313	0.328	0.362
13			0.008	0.035			0.146	0.179			0.259	0.279			
14					0.054	0.090			0.190	0.218			0.282	0.299	0.339
15			0.001	0.015			0.108	0.141			0.225	0.248			
16					0.031	0.060			0.155	0.184			0.253	0.271	0.315
17				0.005			0.078	0.109			0.194	0.218			
18					0.016	0.038			0.125	0.153			0.225	0.245	0.293
19				0.001			0.054	0.082			0.165	0.190			
20					0.007	0.022			0.098	0.126			0.199	0.220	0.271
21				0.000			0.036	0.060			0.140	0.164			
22					0.002	0.012			0.076	0.102			0.175	0.196	0.250
23							0.023	0.043			0.117	0.141			
24					0.001	0.006			0.058	0.082			0.153	0.174	0.230
25							0.014	0.030			0.096	0.120			
26					0.000	0.003			0.043	0.064			0.133	0.154	0.211
27							0.008	0.020			0.079	0.101			
28						0.001			0.031	0.050			0.114	0.135	0.193
29							0.005	0.013			0.063	0.084			
30						0.000			0.022	0.038			0.097	0.118	0.176
31							0.002	0.008			0.050	0.070			
32									0.016	0.029			0.083	0.102	0.159
33							0.001	0.005			0.040	0.057			
34									0.010	0.021			0.070	0.088	0.144
35							0.000	0.003			0.031	0.046			
36									0.007	0.015			0.058	0.076	0.130
37								0.002			0.024	0.037			
38									0.004	0.011			0.048	0.064	0.117
39								0.001			0.018	0.029			
40									0.003	0.007			0.039	0.054	0.104
41								0.000			0.013	0.023			
42									0.002	0.005			0.032	0.046	0.093
43											0.010	0.018			
44									0.001	0.003			0.026	0.038	0.082
45											0.007	0.014			
46									0.000	0.002			0.021	0.032	0.073
47											0.005	0.010			
48										0.001			0.016	0.026	0.064
49											0.003	0.008			
50										0.001			0.013	0.021	0.056

Figure B.1.2. Upper-Tail Probabilities for the Null distribution of Kendall’s S Statistics (continued)

"S"	**Number of Sampling Rounds**														
Value	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**20**
51											0.002	0.006			
52										0.000			0.010	0.017	0.049
53											0.002	0.004			
54													0.008	0.014	0.043
55											0.001	0.003			
56													0.006	0.011	0.037
57											0.001	0.002			
58													0.004	0.009	0.032
59											0.000	0.001			
60													0.003	0.007	0.027
61												0.001			
62													0.002	0.005	0.023
63												0.001			
64													0.001	0.004	0.020
65												0.000			
66													0.001	0.003	0.017
67															
68													0.001	0.002	0.014
69															
70													0.001	0.002	0.012
71															
72													0.001	0.001	0.010
73															
74													0.000	0.001	0.008
75															
76														0.001	0.007
77															
78														0.000	0.006
79															
80															0.005
81															
82															0.004
83															
84															0.003
85															
86															0.002
87															
88															0.002
89															
90															0.002
91															
92															0.001
93															
94															0.001
95															
96															0.001
97															
98															0.001
99															
100															0.000

Figure B.1.3. Mann-Whitney U Trend Test for Plume Stability (Non-parametric Statistical Test)



Module 1: Mann-Whitney U Trend Test for Plume Stability: Non-parametric Statistical Test

(Wilcoxon Rank Sum Test)

Site Name: *ABC Store*
Site Address: *Olympia, WA*
Additional Description: *Demo NA site*

Well (Sampling) Location MW-2

1. Monitoring Well Information: Contaminant Concentration at a well: Quarterly sampling recommended.

			Contaminant of Concern (unit is ug/L)					
Sampling Event	$D_n - D_{n-1}$	Date Sampled	Toluene	Benzene	Ethylbenzene		Naphthalene	MTBE
1st Yr, 1st Qtr		10/14/1993	3.50	9.70	16.00		1.90	11.00
1st Yr, 2nd Qtr	105	1/27/1994	2.90	19.00	15.00		20.00	0.00
1st Yr, 3rd Qtr	118	5/25/1994	2.60	13.00	5.60		3.90	17.00
1st Yr, 4th Qtr	77	8/10/1994	2.40	38.00	6.00		24.50	55.00
2nd Yr, 1st Qtr	85	11/3/1994	2.30	18.00	7.60		65.00	0.50
2nd Yr, 2nd Qtr	106	2/17/1995	3.00	16.00	5.30		15.70	0.50
2nd Yr, 3rd Qtr	90	5/18/1995	1.00	33.00	4.50		28.90	0.50
2nd Yr, 4th Qtr	71	7/28/1995	2.20	28.00	4.60		16.20	0.50

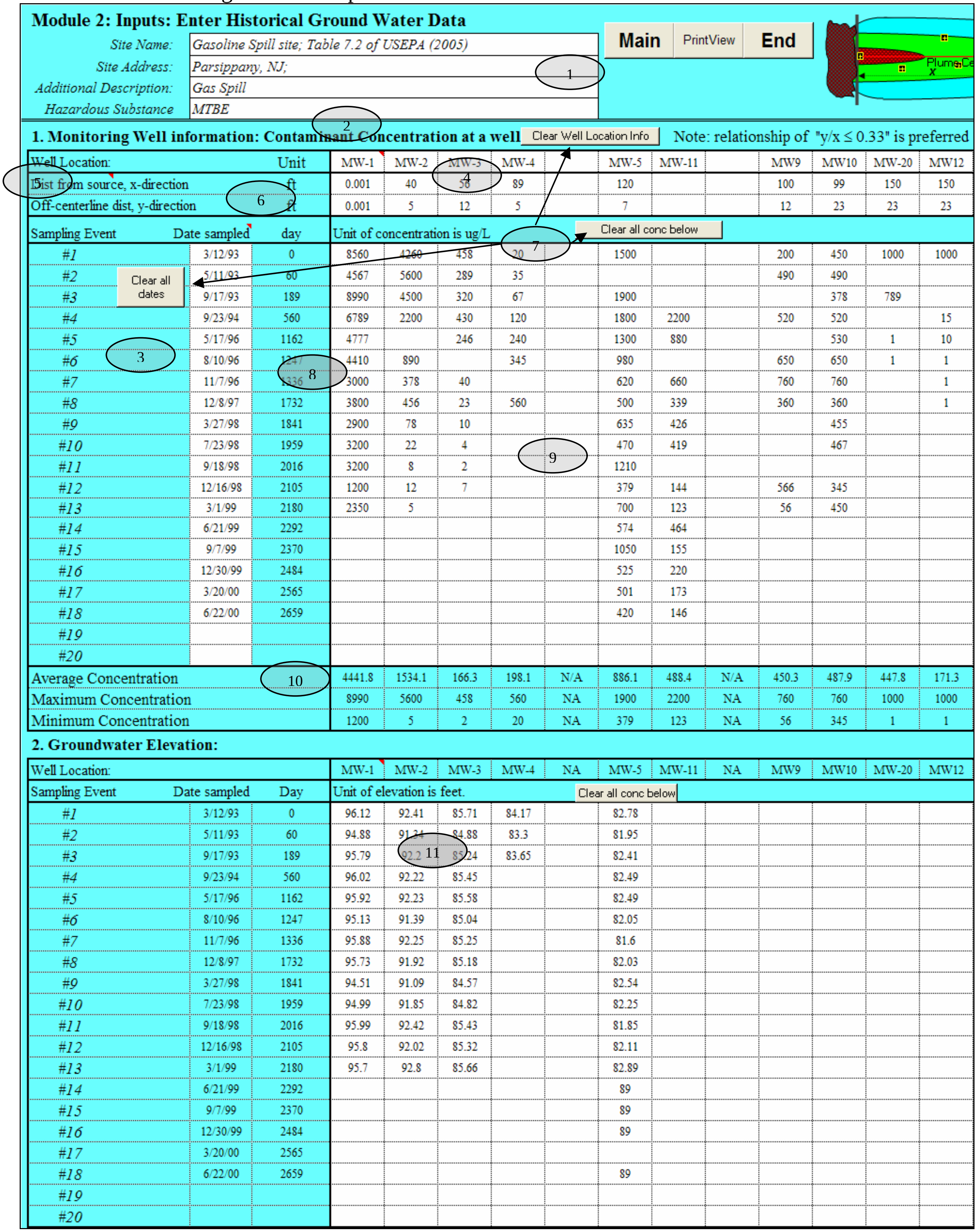
2. Mann-Whitney U Non-parametric Statistical Test Results (@ 90% Confidence Level pre-determined)

U Statistic?	3	10	2	n<8	12	4
Plume Stability?	Shrinking	Undetermined	Shrinking	n<8	Undetermined	Undetermined
Blank If No Errors found				n<8		
DATA FROM QUARTERLY SAMPLING						

3. Temporal Trend: Plot of Concentration vs. Sampling Time

Hazardous substance? **Toluene**
Plume Stability? **Shrinking**

Figure B.2.1. Inputs: Enter Historical Ground Water Data



Module 2: Inputs: Enter Historical Ground Water Data

Site Name:	*Gasoline Spill site; Table 7.2 of USEPA (2005)*
Site Address:	*Parsippany, NJ;*
Additional Description:	*Gas Spill*
Hazardous Substance	*MTBE*

1. Monitoring Well information: Contaminant Concentration at a well

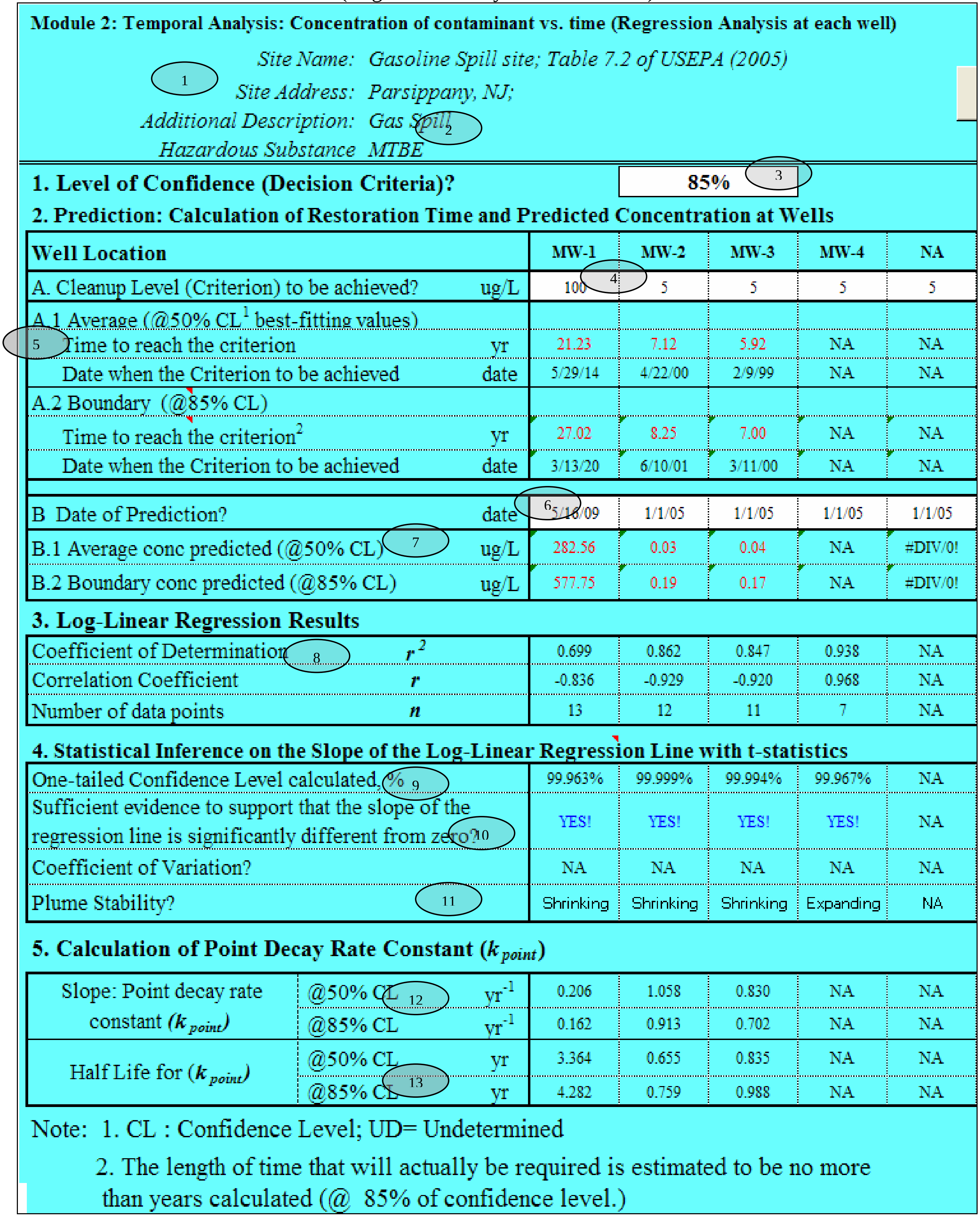
Note: relationship of "y/x ≤ 0.33" is preferred

Well Location:		Unit	MW-1	MW-2	MW-3	MW-4		MW-5	MW-11		MW9	MW10	MW-20	MW12
Dist from source, x-direction		ft	0.001	40	56	89		120			100	99	150	150
Off-centerline dist, y-direction		ft	0.001	5	12	5		7			12	23	23	23
Sampling Event	Date sampled	day	Unit of concentration is ug/L											
#1	3/12/93	0	8560	4260	458	20		1500			200	450	1000	1000
#2	5/11/93	60	4567	5600	289	35					490	490		
#3	9/17/93	189	8990	4500	320	67		1900				378	789	
#4	9/23/94	560	6789	2200	430	120		1800	2200		520	520		15
#5	5/17/96	1162	4777		246	240		1300	880			530	1	10
#6	8/10/96	1247	4410	890		345		980			650	650	1	1
#7	11/7/96	1336	3000	378	40			620	660		760	760		1
#8	12/8/97	1732	3800	456	23	560		500	339		360	360		1
#9	3/27/98	1841	2900	78	10			635	426			455		
#10	7/23/98	1959	3200	22	4			470	419			467		
#11	9/18/98	2016	3200	8	2			1210						
#12	12/16/98	2105	1200	12	7			379	144		566	345		
#13	3/1/99	2180	2350	5				700	123		56	450		
#14	6/21/99	2292						574	464					
#15	9/7/99	2370						1050	155					
#16	12/30/99	2484						525	220					
#17	3/20/00	2565						501	173					
#18	6/22/00	2659						420	146					
#19														
#20														
Average Concentration			4441.8	1534.1	166.3	198.1	N/A	886.1	488.4	N/A	450.3	487.9	447.8	171.3
Maximum Concentration			8990	5600	458	560	NA	1900	2200	NA	760	760	1000	1000
Minimum Concentration			1200	5	2	20	NA	379	123	NA	56	345	1	1

2. Groundwater Elevation:

Well Location:			MW-1	MW-2	MW-3	MW-4	NA	MW-5	MW-11	NA	MW9	MW10	MW-20	MW12
Sampling Event	Date sampled	Day	Unit of elevation is feet.											
#1	3/12/93	0	96.12	92.41	85.71	84.17		82.78						
#2	5/11/93	60	94.88	91.34	84.88	83.3		81.95						
#3	9/17/93	189	95.79	92.2	85.24	83.65		82.41						
#4	9/23/94	560	96.02	92.22	85.45			82.49						
#5	5/17/96	1162	95.92	92.23	85.58			82.49						
#6	8/10/96	1247	95.13	91.39	85.04			82.05						
#7	11/7/96	1336	95.88	92.25	85.25			81.6						
#8	12/8/97	1732	95.73	91.92	85.18			82.03						
#9	3/27/98	1841	94.51	91.09	84.57			82.54						
#10	7/23/98	1959	94.99	91.85	84.82			82.25						
#11	9/18/98	2016	95.99	92.42	85.43			81.85						
#12	12/16/98	2105	95.8	92.02	85.32			82.11						
#13	3/1/99	2180	95.7	92.8	85.66			82.89						
#14	6/21/99	2292						89						
#15	9/7/99	2370						89						
#16	12/30/99	2484						89						
#17	3/20/00	2565												
#18	6/22/00	2659						89						
#19														
#20														

Figure B.2.2. Temporal Analysis: concentration of contaminant vs. time at wells
(Regression Analysis for each well)



Module 2: Temporal Analysis: Concentration of contaminant vs. time (Regression Analysis at each well)

Site Name: *Gasoline Spill site; Table 7.2 of USEPA (2005)*
Site Address: *Parsippany, NJ;*
Additional Description: *Gas Spill*
Hazardous Substance *MTBE*

1. Level of Confidence (Decision Criteria)? **85%**

2. Prediction: Calculation of Restoration Time and Predicted Concentration at Wells

Well Location		MW-1	MW-2	MW-3	MW-4	NA
A. Cleanup Level (Criterion) to be achieved?	ug/L	100	5	5	5	5
A.1 Average (@50% CL[1] best-fitting values)						
Time to reach the criterion	yr	21.23	7.12	5.92	NA	NA
Date when the Criterion to be achieved	date	5/29/14	4/22/00	2/9/99	NA	NA
A.2 Boundary (@85% CL)						
Time to reach the criterion[2]	yr	27.02	8.25	7.00	NA	NA
Date when the Criterion to be achieved	date	3/13/20	6/10/01	3/11/00	NA	NA
B Date of Prediction?	date	5/16/09	1/1/05	1/1/05	1/1/05	1/1/05
B.1 Average conc predicted (@50% CL)	ug/L	282.56	0.03	0.04	NA	#DIV/0!
B.2 Boundary conc predicted (@85% CL)	ug/L	577.75	0.19	0.17	NA	#DIV/0!

3. Log-Linear Regression Results

		MW-1	MW-2	MW-3	MW-4	NA
Coefficient of Determination	r^2	0.699	0.862	0.847	0.938	NA
Correlation Coefficient	r	-0.836	-0.929	-0.920	0.968	NA
Number of data points	n	13	12	11	7	NA

4. Statistical Inference on the Slope of the Log-Linear Regression Line with t-statistics

	MW-1	MW-2	MW-3	MW-4	NA
One-tailed Confidence Level calculated, %	99.963%	99.999%	99.994%	99.967%	NA
Sufficient evidence to support that the slope of the regression line is significantly different from zero?	YES!	YES!	YES!	YES!	NA
Coefficient of Variation?	NA	NA	NA	NA	NA
Plume Stability?	Shrinking	Shrinking	Shrinking	Expanding	NA

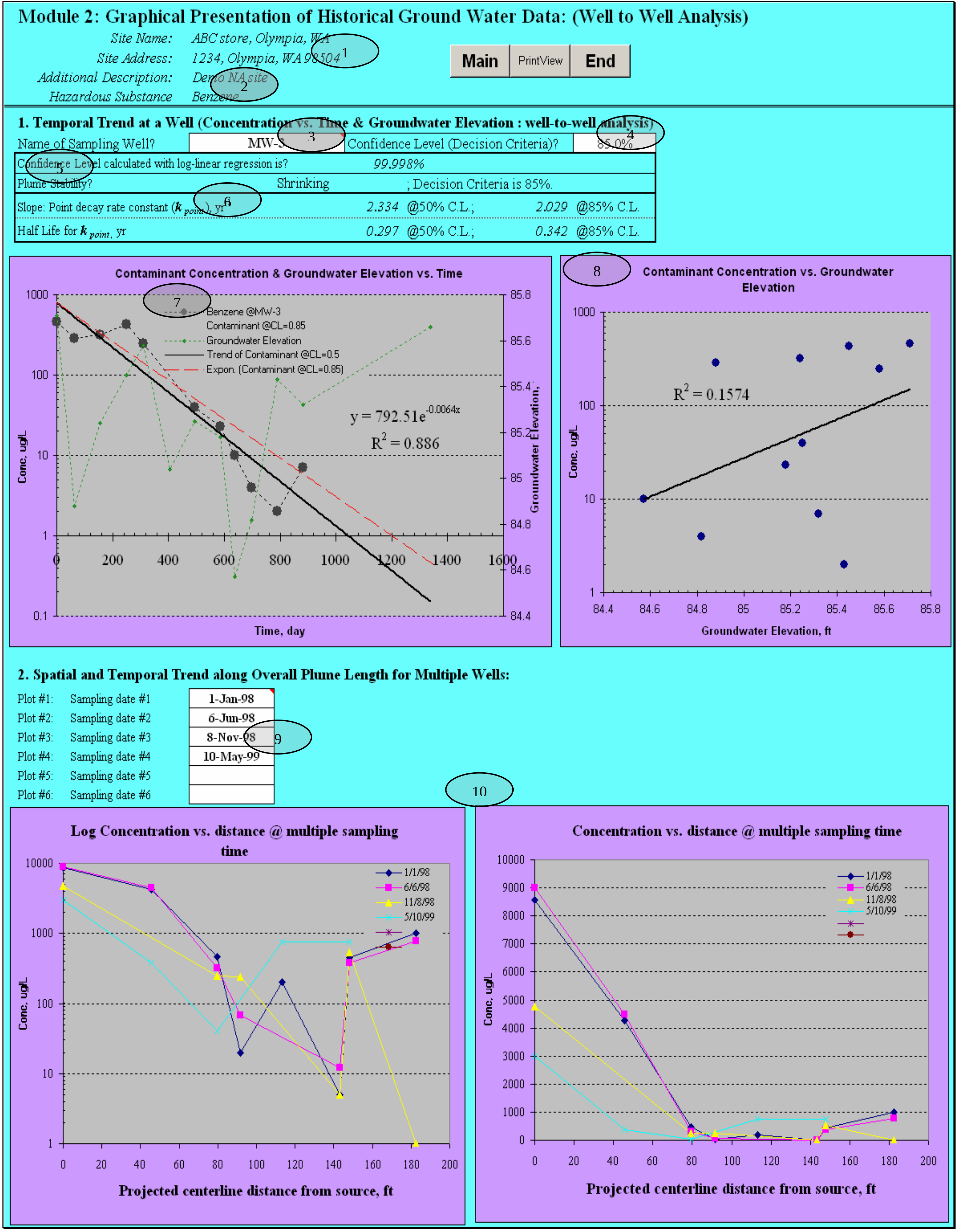
5. Calculation of Point Decay Rate Constant (k_{point})

			MW-1	MW-2	MW-3	MW-4	NA
Slope: Point decay rate constant (k_{point})	@50% CL	yr^{-1}	0.206	1.058	0.830	NA	NA
	@85% CL	yr^{-1}	0.162	0.913	0.702	NA	NA
Half Life for (k_{point})	@50% CL	yr	3.364	0.655	0.835	NA	NA
	@85% CL	yr	4.282	0.759	0.988	NA	NA

Note: 1. CL : Confidence Level; UD= Undetermined

2. The length of time that will actually be required is estimated to be no more than years calculated (@ 85% of confidence level.)

Figure B.2.3. Graphical Presentation of Historical Ground Water Data (Well to Well Analysis)



Module 2: Graphical Presentation of Historical Ground Water Data: (Well to Well Analysis)

Site Name: ABC store, Olympia, WA
Site Address: 1234, Olympia, WA 98504
Additional Description: Demo NA site
Hazardous Substance Benzene

1. Temporal Trend at a Well (Concentration vs. Time & Groundwater Elevation : well-to-well analysis)

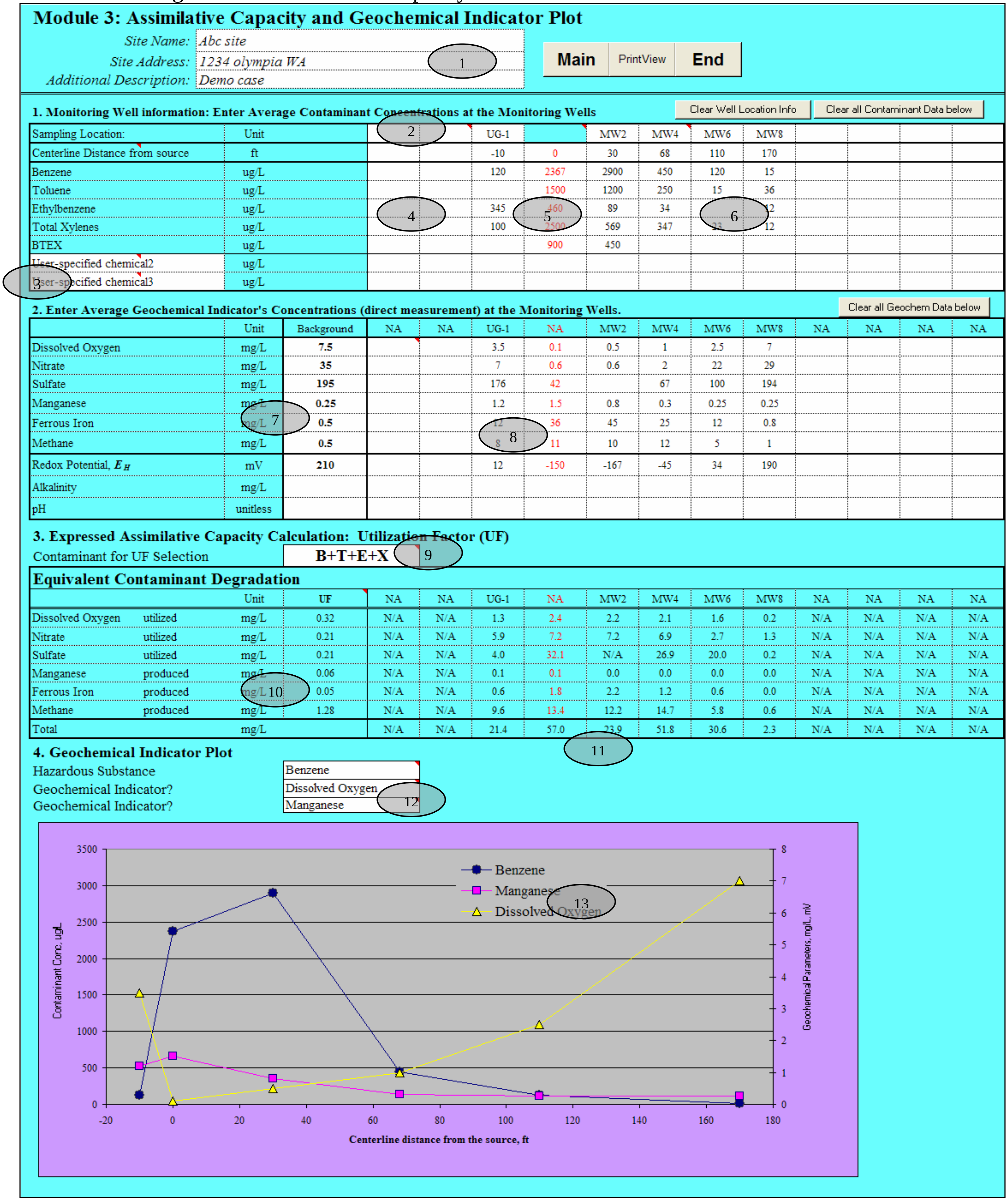
Name of Sampling Well? MW-3
Confidence Level (Decision Criteria)? 85.0%

Confidence Level calculated with log-linear regression is?	99.998%			
Plume Stability?	Shrinking	; Decision Criteria is 85%.		
Slope: Point decay rate constant (k_{point}), yr	2.334	@50% C.L.;	2.029	@85% C.L.
Half Life for k_{point}, yr	0.297	@50% C.L.;	0.342	@85% C.L.

2. Spatial and Temporal Trend along Overall Plume Length for Multiple Wells:

Plot #1:	Sampling date #1	1-Jan-98
Plot #2:	Sampling date #2	6-Jun-98
Plot #3:	Sampling date #3	8-Nov-98
Plot #4:	Sampling date #4	10-May-99
Plot #5:	Sampling date #5	
Plot #6:	Sampling date #6	

Figure B.3. Assimilative Capacity Calculation and Geochemical Indicator Plot



Module 3: Assimilative Capacity and Geochemical Indicator Plot

Site Name: Abc site
Site Address: 1234 olympia WA
Additional Description: Demo case

1. Monitoring Well information: Enter Average Contaminant Concentrations at the Monitoring Wells

Sampling Location:	Unit			UG-1		MW2	MW4	MW6	MW8				
Centerline Distance from source	ft			-10	0	30	68	110	170				
Benzene	ug/L			120	2367	2900	450	120	15				
Toluene	ug/L				1500	1200	250	15	36				
Ethylbenzene	ug/L			345	460	89	34		12				
Total Xylenes	ug/L			100	2500	569	347	23	12				
BTEX	ug/L				900	450							
User-specified chemical2	ug/L												
User-specified chemical3	ug/L												

2. Enter Average Geochemical Indicator's Concentrations (direct measurement) at the Monitoring Wells.

	Unit	Background	NA	NA	UG-1	NA	MW2	MW4	MW6	MW8	NA	NA	NA	NA
Dissolved Oxygen	mg/L	**7.5**			3.5	0.1	0.5	1	2.5	7				
Nitrate	mg/L	**35**			7	0.6	0.6	2	22	29				
Sulfate	mg/L	**195**			176	42		67	100	194				
Manganese	mg/L	**0.25**			1.2	1.5	0.8	0.3	0.25	0.25				
Ferrous Iron	mg/L	**0.5**			12	36	45	25	12	0.8				
Methane	mg/L	**0.5**			8	11	10	12	5	1				
Redox Potential, E_H	mV	**210**			12	-150	-167	-45	34	190				
Alkalinity	mg/L													
pH	unitless													

3. Expressed Assimilative Capacity Calculation: Utilization Factor (UF)

Contaminant for UF Selection: **B+T+E+X**

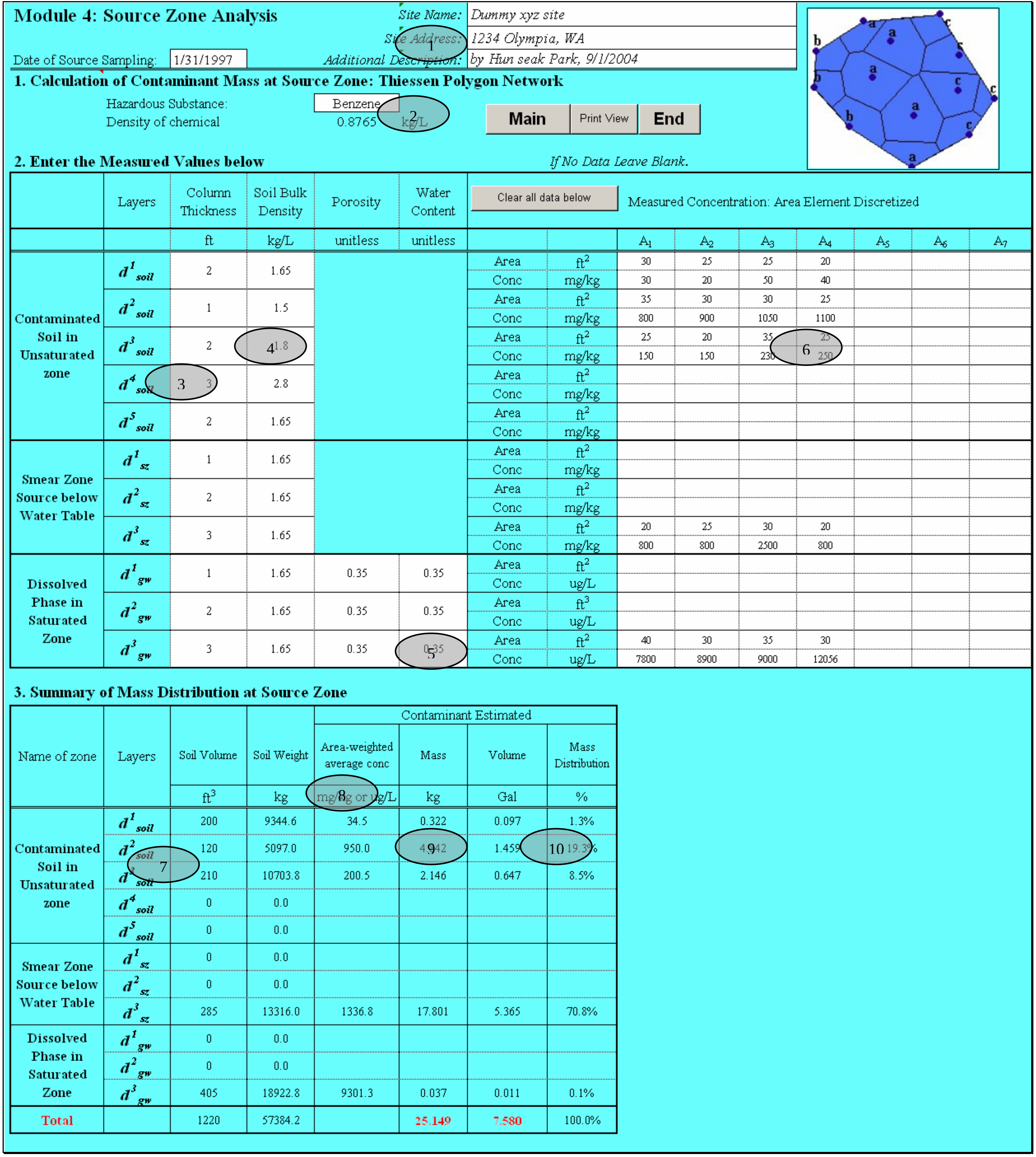
Equivalent Contaminant Degradation

		Unit	UF	NA	NA	UG-1	NA	MW2	MW4	MW6	MW8	NA	NA	NA	NA
Dissolved Oxygen	utilized	mg/L	0.32	N/A	N/A	1.3	2.4	2.2	2.1	1.6	0.2	N/A	N/A	N/A	N/A
Nitrate	utilized	mg/L	0.21	N/A	N/A	5.9	7.2	7.2	6.9	2.7	1.3	N/A	N/A	N/A	N/A
Sulfate	utilized	mg/L	0.21	N/A	N/A	4.0	32.1	N/A	26.9	20.0	0.2	N/A	N/A	N/A	N/A
Manganese	produced	mg/L	0.06	N/A	N/A	0.1	0.1	0.0	0.0	0.0	0.0	N/A	N/A	N/A	N/A
Ferrous Iron	produced	mg/L	0.05	N/A	N/A	0.6	1.8	2.2	1.2	0.6	0.0	N/A	N/A	N/A	N/A
Methane	produced	mg/L	1.28	N/A	N/A	9.6	13.4	12.2	14.7	5.8	0.6	N/A	N/A	N/A	N/A
Total		mg/L		N/A	N/A	21.4	57.0	23.9	51.8	30.6	2.3	N/A	N/A	N/A	N/A

4. Geochemical Indicator Plot

Hazardous Substance: Benzene
Geochemical Indicator?: Dissolved Oxygen
Geochemical Indicator?: Manganese

Figure B.4. Source Zone Analysis



Module 4: Source Zone Analysis

Site Name: *Dummy xyz site*
Site Address: *1234 Olympia, WA*
Date of Source Sampling: 1/31/1997
Additional Description: *by Hun seak Park, 9/1/2004*

1. Calculation of Contaminant Mass at Source Zone: Thiessen Polygon Network

Hazardous Substance: Benzene
Density of chemical 0.8765 kg/L

2. Enter the Measured Values below

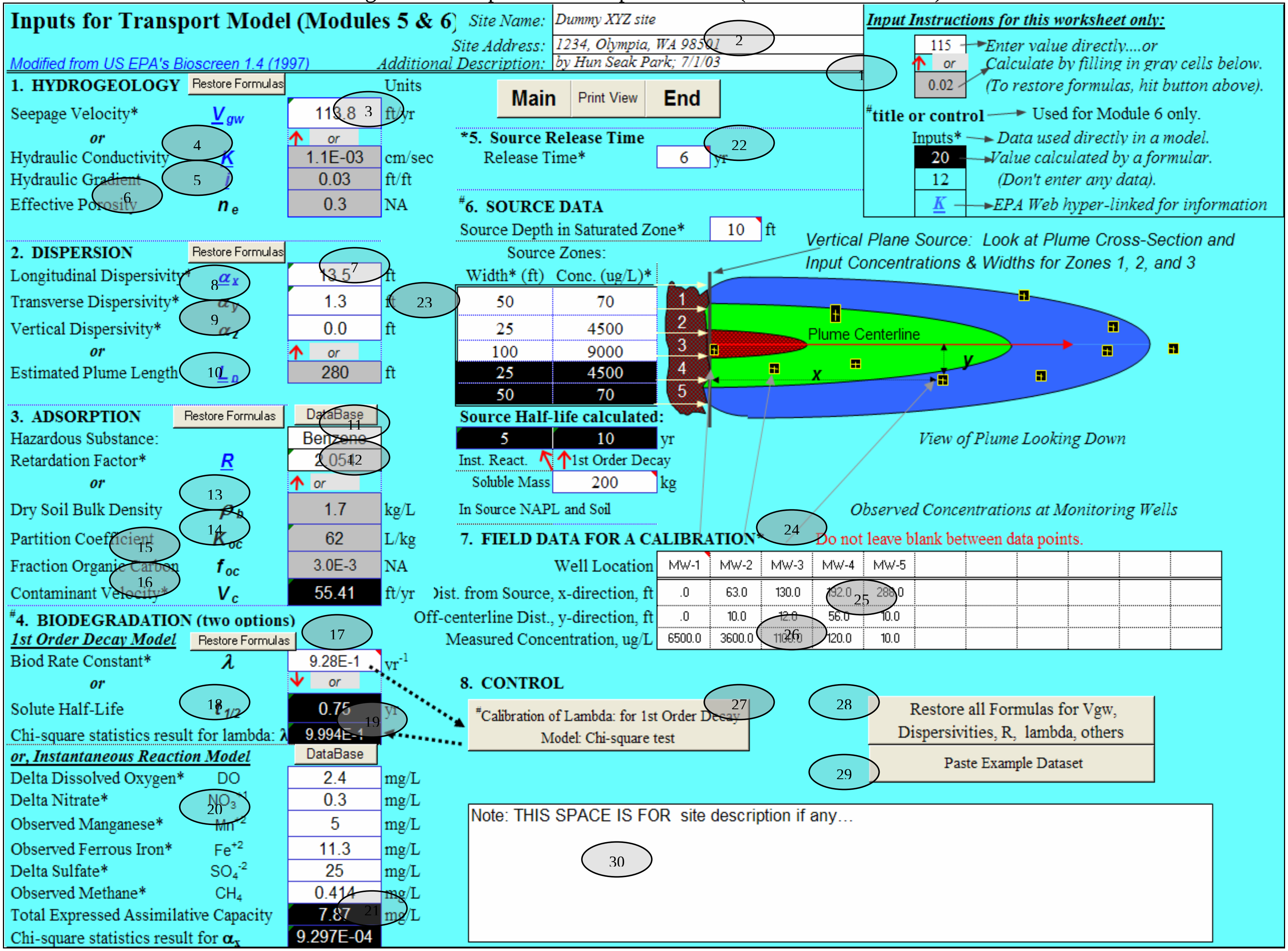
If No Data Leave Blank.

	Layers	Column Thickness	Soil Bulk Density	Porosity	Water Content	Measured Concentration: Area Element Discretized								
		ft	kg/L	unitless	unitless			A_1	A_2	A_3	A_4	A_5	A_6	A_7
Contaminated Soil in Unsaturated zone	d^1_{soil}	2	1.65			Area	ft^2	30	25	25	20			
						Conc	mg/kg	30	20	50	40			
	d^2_{soil}	1	1.5			Area	ft^2	35	30	30	25			
						Conc	mg/kg	800	900	1050	1100			
	d^3_{soil}	2	1.8			Area	ft^2	25	20	35	25			
						Conc	mg/kg	150	150	230	250			
	d^4_{soil}	3	2.8			Area	ft^2							
						Conc	mg/kg							
	d^5_{soil}	2	1.65			Area	ft^2							
						Conc	mg/kg							
Smear Zone Source below Water Table	d^1_{sz}	1	1.65			Area	ft^2							
						Conc	mg/kg							
	d^2_{sz}	2	1.65			Area	ft^2							
						Conc	mg/kg							
	d^3_{sz}	3	1.65			Area	ft^2	20	25	30	20			
						Conc	mg/kg	800	800	2500	800			
Dissolved Phase in Saturated Zone	d^1_{gw}	1	1.65	0.35	0.35	Area	ft^2							
						Conc	ug/L							
	d^2_{gw}	2	1.65	0.35	0.35	Area	ft^3							
						Conc	ug/L							
	d^3_{gw}	3	1.65	0.35	0.35	Area	ft^2	40	30	35	30			
						Conc	ug/L	7800	8900	9000	12056			

3. Summary of Mass Distribution at Source Zone

Name of zone	Layers	Soil Volume	Soil Weight	Contaminant Estimated			
				Area-weighted average conc	Mass	Volume	Mass Distribution
		ft^3	kg	mg/kg or ug/L	kg	Gal	%
Contaminated Soil in Unsaturated zone	d^1_{soil}	200	9344.6	34.5	0.322	0.097	1.3%
	d^2_{soil}	120	5097.0	950.0	4.842	1.459	19.3%
	d^3_{soil}	210	10703.8	200.5	2.146	0.647	8.5%
	d^4_{soil}	0	0.0				
	d^5_{soil}	0	0.0				
Smear Zone Source below Water Table	d^1_{sz}	0	0.0				
	d^2_{sz}	0	0.0				
	d^3_{sz}	285	13316.0	1336.8	17.801	5.365	70.8%
Dissolved Phase in Saturated Zone	d^1_{gw}	0	0.0				
	d^2_{gw}	0	0.0				
	d^3_{gw}	405	18922.8	9301.3	0.037	0.011	0.1%
Total		1220	57384.2		**25.149**	**7.580**	100.0%

Figure B.5.1 Inputs for Transport Models (for Modules 5 and 6)



Inputs for Transport Model (Modules 5 & 6)

Modified from US EPA's Bioscreen 1.4 (1997)

Site Name: Dummy XYZ site
Site Address: 1234, Olympia, WA 98501
Additional Description: by Hun Seak Park; 7/1/03

1. HYDROGEOLOGY

			Units
Seepage Velocity*	V_{gw}	113.8	ft/yr
or		or	
Hydraulic Conductivity	K	1.1E-03	cm/sec
Hydraulic Gradient	i	0.03	ft/ft
Effective Porosity	n_e	0.3	NA

2. DISPERSION

Longitudinal Dispersivity*	α_x	13.5	ft
Transverse Dispersivity*	α_y	1.3	ft
Vertical Dispersivity*	α_z	0.0	ft
or		or	
Estimated Plume Length	L_p	280	ft

3. ADSORPTION

Hazardous Substance:		Benzene	
Retardation Factor*	R	2.054	
or		or	
Dry Soil Bulk Density	ρ_b	1.7	kg/L
Partition Coefficient	K_{oc}	62	L/kg
Fraction Organic Carbon	f_{oc}	3.0E-3	NA
Contaminant Velocity*	V_c	55.41	ft/yr

#4. BIODEGRADATION (two options)

1st Order Decay Model

Biod Rate Constant*	λ	9.28E-1	yr^{-1}
or		or	
Solute Half-Life	$t_{1/2}$	0.75	yr
Chi-square statistics result for lambda: λ		9.994E-1	

or, Instantaneous Reaction Model

Delta Dissolved Oxygen*	DO	2.4	mg/L
Delta Nitrate*	NO_3^{-1}	0.3	mg/L
Observed Manganese*	Mn^{+2}	5	mg/L
Observed Ferrous Iron*	Fe^{+2}	11.3	mg/L
Delta Sulfate*	SO_4^{-2}	25	mg/L
Observed Methane*	CH_4	0.414	mg/L
Total Expressed Assimilative Capacity		7.87	mg/L
Chi-square statistics result for α_x		9.297E-04	

***5. Source Release Time**

Release Time* 6 yr

#6. SOURCE DATA

Source Depth in Saturated Zone* 10 ft

Source Zones:

Width* (ft)	Conc. (ug/L)*
50	70
25	4500
100	9000
25	4500
50	70

Source Half-life calculated:

5	10	yr
Inst. React.	1st Order Decay	
Soluble Mass	200	kg

In Source NAPL and Soil

Vertical Plane Source: Look at Plume Cross-Section and Input Concentrations & Widths for Zones 1, 2, and 3

View of Plume Looking Down

Observed Concentrations at Monitoring Wells

7. FIELD DATA FOR A CALIBRATION*

Do not leave blank between data points.

Well Location	MW-1	MW-2	MW-3	MW-4	MW-5						
Dist. from Source, x-direction, ft	.0	63.0	130.0	192.0	288.0						
Off-centerline Dist., y-direction, ft	.0	10.0	12.0	56.0	10.0						
Measured Concentration, ug/L	6500.0	3600.0	1100.0	120.0	10.0						

8. CONTROL

#Calibration of Lambda: for 1st Order Decay Model: Chi-square test

Restore all Formulas for Vgw, Dispersivities, R, lambda, others

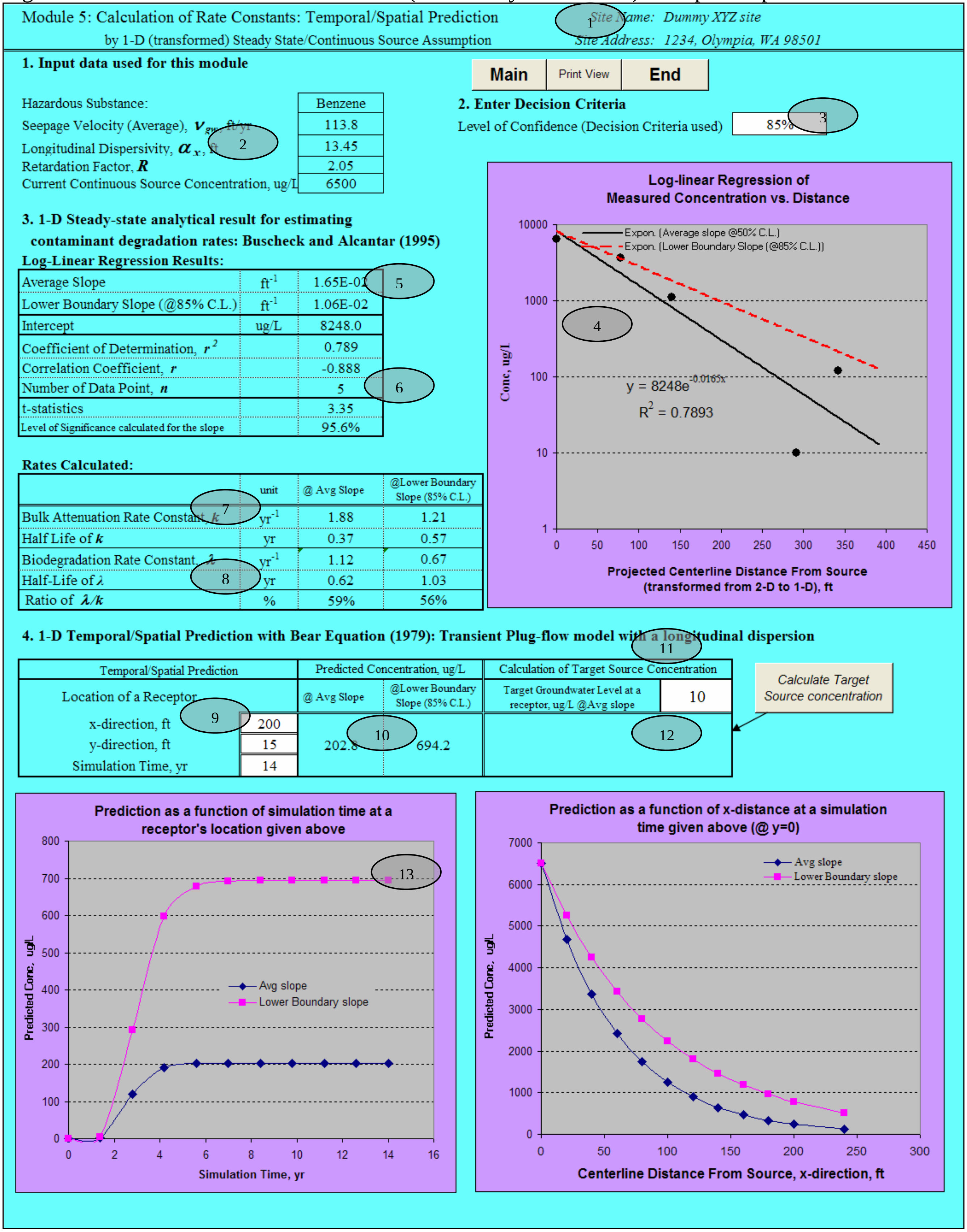
Paste Example Dataset

Note: THIS SPACE IS FOR site description if any…

Input Instructions for this worksheet only:

115 → Enter value directly....or
or Calculate by filling in gray cells below.
0.02 (To restore formulas, hit button above).
#title or control → Used for Module 6 only.
Inputs* → Data used directly in a model.
20 → Value calculated by a formular.
12 (Don't enter any data).
K → EPA Web hyper-linked for information

Figure B.5.2 Calculation of Rate Constants (1-D Steady State Mode): Temporal/Spatial Prediction



Module 5: Calculation of Rate Constants: Temporal/Spatial Prediction
by 1-D (transformed) Steady State/Continuous Source Assumption

Site Name: *Dummy XYZ site*
Site Address: *1234, Olympia, WA 98501*

1. Input data used for this module

Hazardous Substance:	Benzene
Seepage Velocity (Average), v_{gw}, ft/yr	113.8
Longitudinal Dispersivity, α_x, ft	13.45
Retardation Factor, R	2.05
Current Continuous Source Concentration, ug/L	6500

2. Enter Decision Criteria

Level of Confidence (Decision Criteria used): 85%

3. 1-D Steady-state analytical result for estimating contaminant degradation rates: Buscheck and Alcantar (1995)

Log-Linear Regression Results:

Average Slope	ft^{-1}	1.65E-02
Lower Boundary Slope (@85% C.L.)	ft^{-1}	1.06E-02
Intercept	ug/L	8248.0
Coefficient of Determination, r^2		0.789
Correlation Coefficient, r		-0.888
Number of Data Point, n		5
t-statistics		3.35
Level of Significance calculated for the slope		95.6%

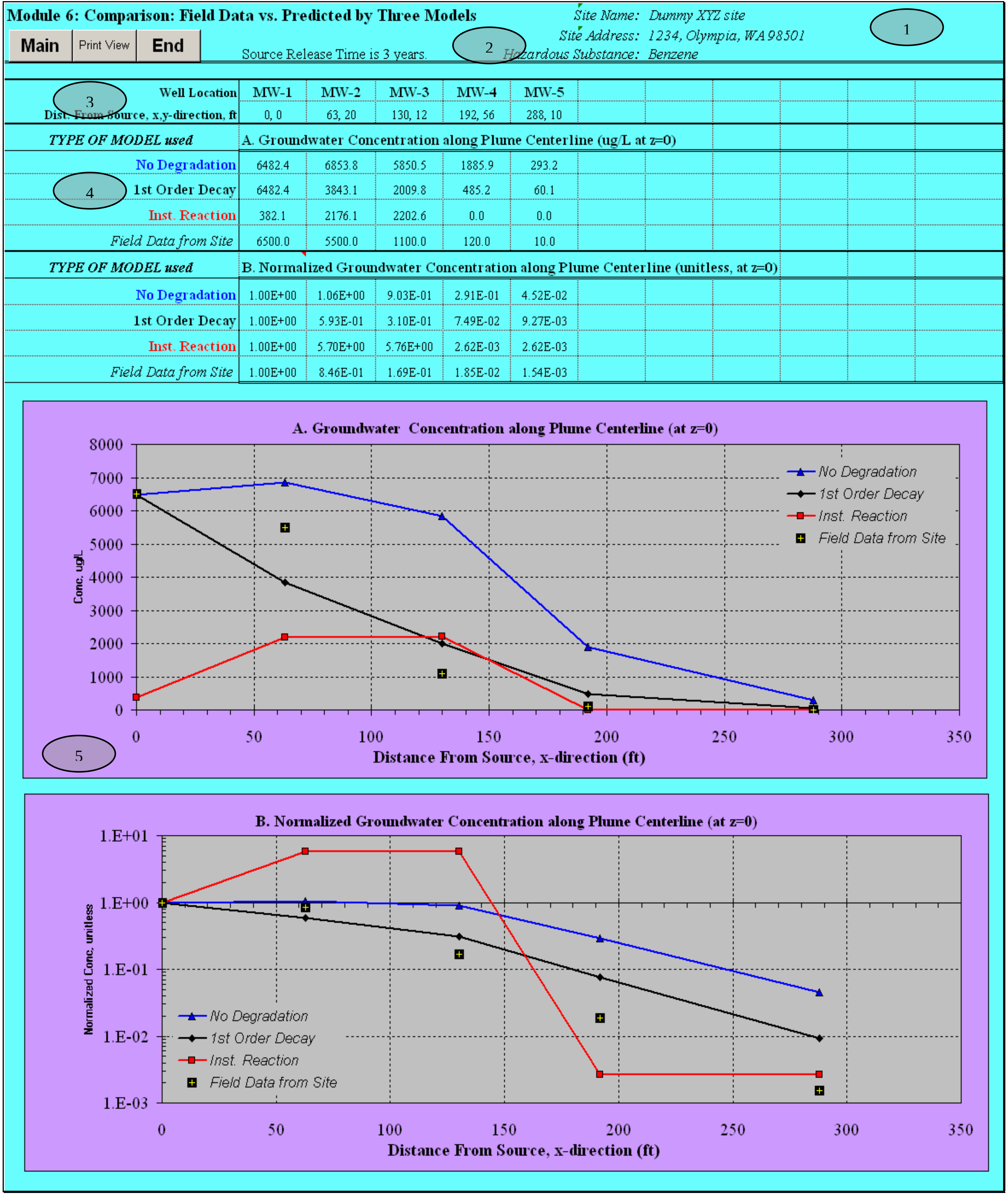
Rates Calculated:

	unit	@ Avg Slope	@Lower Boundary Slope (85% C.L.)
Bulk Attenuation Rate Constant, k	yr^{-1}	1.88	1.21
Half Life of k	yr	0.37	0.57
Biodegradation Rate Constant, λ	yr^{-1}	1.12	0.67
Half-Life of λ	yr	0.62	1.03
Ratio of λ/k	%	59%	56%

4. 1-D Temporal/Spatial Prediction with Bear Equation (1979): Transient Plug-flow model with a longitudinal dispersion

Temporal/Spatial Prediction		Predicted Concentration, ug/L		Calculation of Target Source Concentration	
Location of a Receptor		@ Avg Slope	@Lower Boundary Slope (85% C.L.)	Target Groundwater Level at a receptor, ug/L @Avg slope	10
x-direction, ft	200	202.8	694.2		
y-direction, ft	15				
Simulation Time, yr	14				

Figure B.6.1. Comparison: Field Data vs. Predicted by Three Models



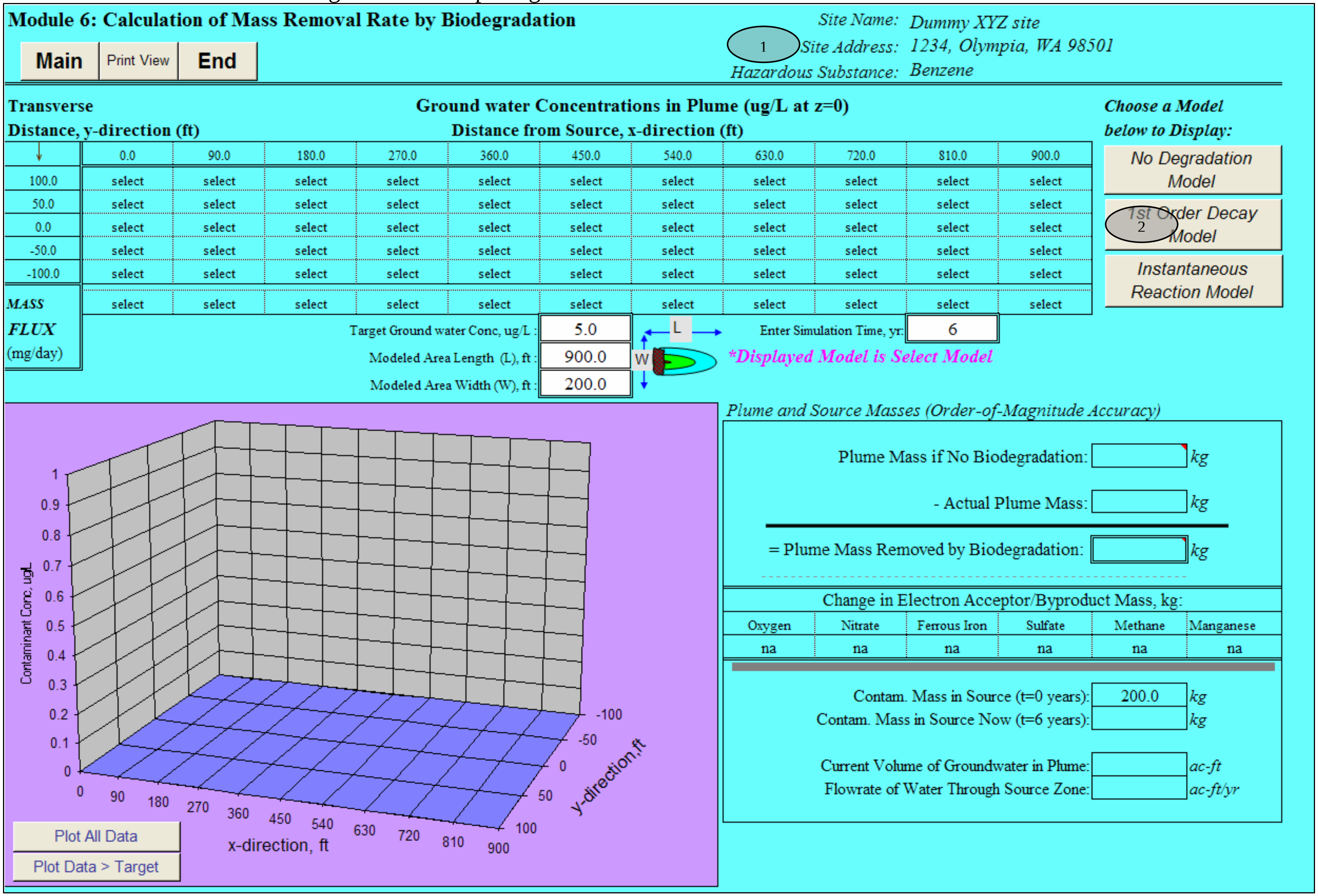
Module 6: Comparison: Field Data vs. Predicted by Three Models

Site Name: Dummy XYZ site
Site Address: 1234, Olympia, WA 98501
Hazardous Substance: Benzene

Source Release Time is 3 years.

Well Location	MW-1	MW-2	MW-3	MW-4	MW-5
Dist. From Source, x,y-direction, ft	0, 0	63, 20	130, 12	192, 56	288, 10
TYPE OF MODEL used	A. Groundwater Concentration along Plume Centerline (ug/L at z=0)				
No Degradation	6482.4	6853.8	5850.5	1885.9	293.2
1st Order Decay	6482.4	3843.1	2009.8	485.2	60.1
Inst. Reaction	382.1	2176.1	2202.6	0.0	0.0
Field Data from Site	6500.0	5500.0	1100.0	120.0	10.0
TYPE OF MODEL used	B. Normalized Groundwater Concentration along Plume Centerline (unitless, at z=0)				
No Degradation	1.00E+00	1.06E+00	9.03E-01	2.91E-01	4.52E-02
1st Order Decay	1.00E+00	5.93E-01	3.10E-01	7.49E-02	9.27E-03
Inst. Reaction	1.00E+00	5.70E+00	5.76E+00	2.62E-03	2.62E-03
Field Data from Site	1.00E+00	8.46E-01	1.69E-01	1.85E-02	1.54E-03

Figure B.6.2.a. Opening worksheet: Calculation of Mass Removal Rate



Module 6: Calculation of Mass Removal Rate by Biodegradation

Site Name: *Dummy XYZ site*
Site Address: *1234, Olympia, WA 98501*
Hazardous Substance: *Benzene*

Ground water Concentrations in Plume (ug/L at z=0)

Transverse Distance, y-direction (ft) ↓	**Distance from Source, x-direction (ft)** 0.0	90.0	180.0	270.0	360.0	450.0	540.0	630.0	720.0	810.0	900.0
100.0	select	select	select	select	select	select	select	select	select	select	select
50.0	select	select	select	select	select	select	select	select	select	select	select
0.0	select	select	select	select	select	select	select	select	select	select	select
-50.0	select	select	select	select	select	select	select	select	select	select	select
-100.0	select	select	select	select	select	select	select	select	select	select	select
MASS FLUX (mg/day)	select	select	select	select	select	select	select	select	select	select	select

Target Ground water Conc, ug/L : 5.0
Modeled Area Length (L), ft : 900.0
Modeled Area Width (W), ft : 200.0
Enter Simulation Time, yr: 6

Choose a Model below to Display:

**Displayed Model is Select Model*

Plume and Source Masses (Order-of-Magnitude Accuracy)

Plume Mass if No Biodegradation: *kg*
- Actual Plume Mass: *kg*
= Plume Mass Removed by Biodegradation: *kg*

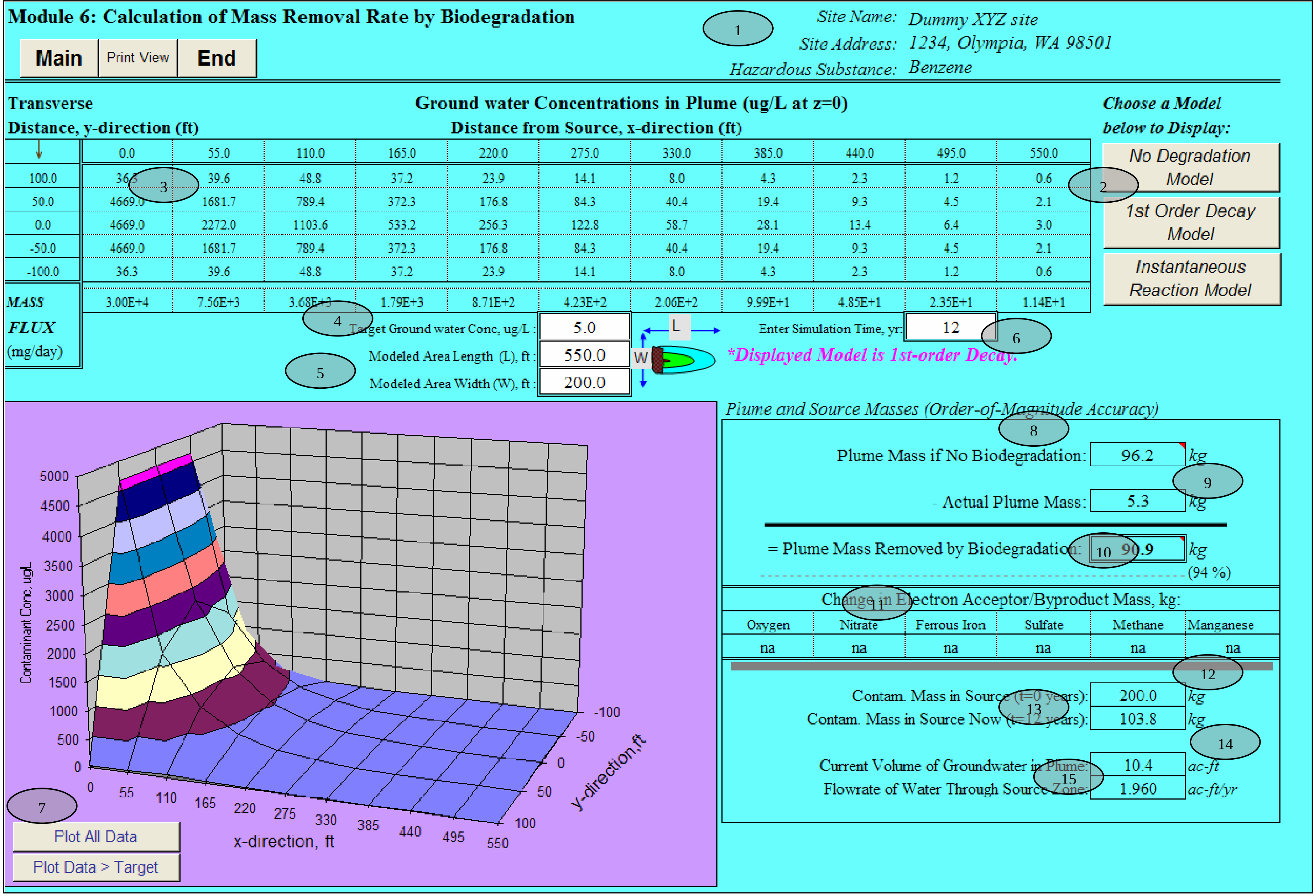
Change in Electron Acceptor/Byproduct Mass, kg:

Oxygen	Nitrate	Ferrous Iron	Sulfate	Methane	Manganese
na	na	na	na	na	na

Contam. Mass in Source (t=0 years): 200.0 *kg*
Contam. Mass in Source Now (t=6 years): *kg*

Current Volume of Groundwater in Plume: *ac-ft*
Flowrate of Water Through Source Zone: *ac-ft/yr*

Figure B.6.2.b. Calculation of Mass Removal Rate by 1st-order Decay Model



Module 6: Calculation of Mass Removal Rate by Biodegradation

Site Name: *Dummy XYZ site*
Site Address: *1234, Olympia, WA 98501*
Hazardous Substance: *Benzene*

Transverse Distance, y-direction (ft)

Ground water Concentrations in Plume (ug/L at z=0)
Distance from Source, x-direction (ft)

↓	0.0	55.0	110.0	165.0	220.0	275.0	330.0	385.0	440.0	495.0	550.0
100.0	36.3	39.6	48.8	37.2	23.9	14.1	8.0	4.3	2.3	1.2	0.6
50.0	4669.0	1681.7	789.4	372.3	176.8	84.3	40.4	19.4	9.3	4.5	2.1
0.0	4669.0	2272.0	1103.6	533.2	256.3	122.8	58.7	28.1	13.4	6.4	3.0
-50.0	4669.0	1681.7	789.4	372.3	176.8	84.3	40.4	19.4	9.3	4.5	2.1
-100.0	36.3	39.6	48.8	37.2	23.9	14.1	8.0	4.3	2.3	1.2	0.6
MASS FLUX (mg/day)	3.00E+4	7.56E+3	3.68E+3	1.79E+3	8.71E+2	4.23E+2	2.06E+2	9.99E+1	4.85E+1	2.35E+1	1.14E+1

Choose a Model below to Display:

- No Degradation Model
- 1st Order Decay Model
- Instantaneous Reaction Model

Target Ground water Conc, ug/L : 5.0
Modeled Area Length (L), ft : 550.0
Modeled Area Width (W), ft : 200.0
Enter Simulation Time, yr: 12

**Displayed Model is 1st-order Decay.*

Plume and Source Masses (Order-of-Magnitude Accuracy)

Plume Mass if No Biodegradation: 96.2 *kg*
\- Actual Plume Mass: 5.3 *kg*
= Plume Mass Removed by Biodegradation: 90.9 *kg*
(94 %)

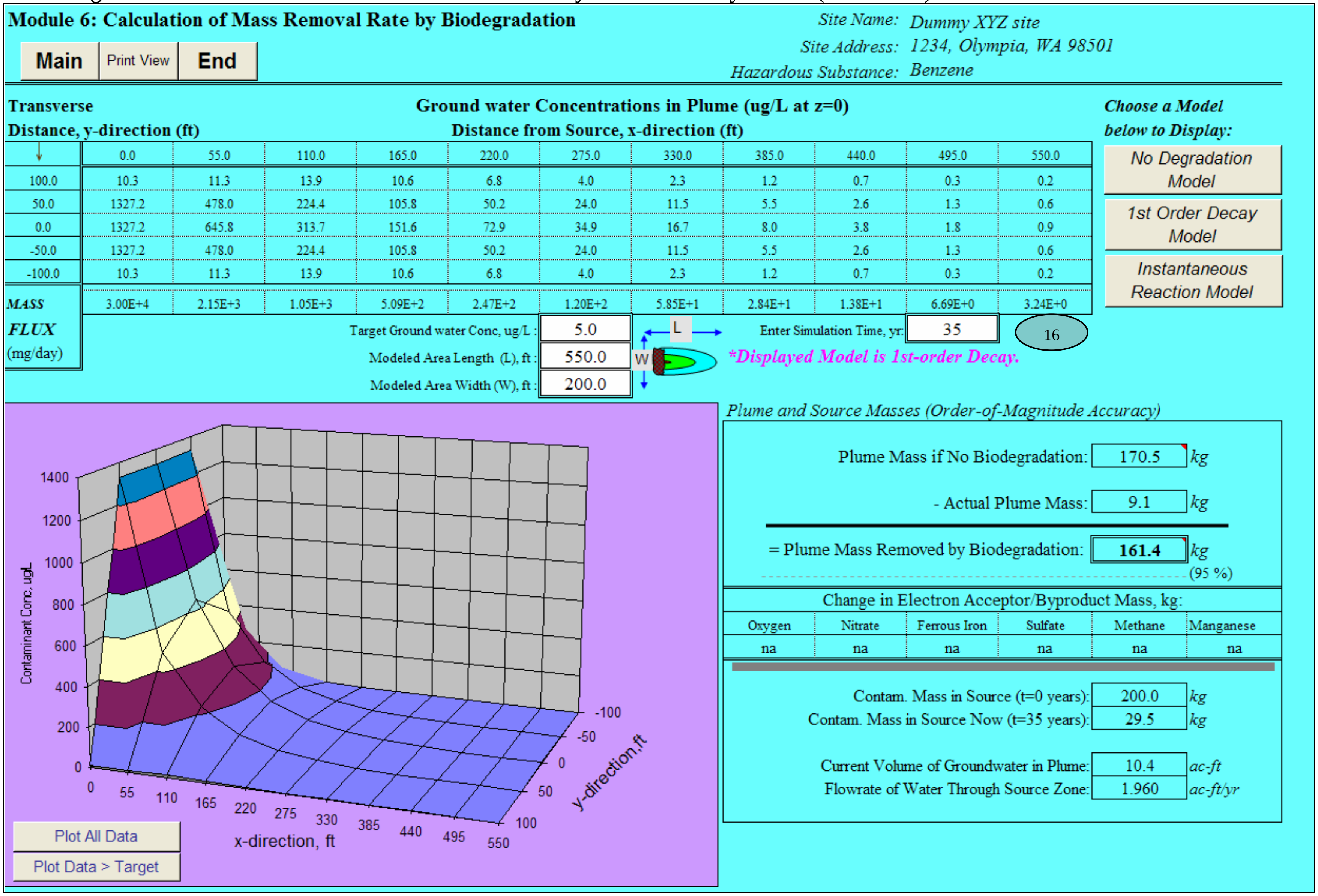
Change in Electron Acceptor/Byproduct Mass, kg:

Oxygen	Nitrate	Ferrous Iron	Sulfate	Methane	Manganese
na	na	na	na	na	na

Contam. Mass in Source (t=0 years): 200.0 *kg*
Contam. Mass in Source Now (t=12 years): 103.8 *kg*

Current Volume of Groundwater in Plume: 10.4 *ac-ft*
Flowrate of Water Through Source Zone: 1.960 *ac-ft/yr*

Figure B.6.2.b. Calculation of Mass Removal Rate by 1st-order Decay Model (Continued): with different simulation time



Module 6: Calculation of Mass Removal Rate by Biodegradation

Site Name: *Dummy XYZ site*
Site Address: *1234, Olympia, WA 98501*
Hazardous Substance: *Benzene*

Ground water Concentrations in Plume (ug/L at z=0)

Distance from Source, x-direction (ft)

Transverse Distance, y-direction (ft) ↓	0.0	55.0	110.0	165.0	220.0	275.0	330.0	385.0	440.0	495.0	550.0
100.0	10.3	11.3	13.9	10.6	6.8	4.0	2.3	1.2	0.7	0.3	0.2
50.0	1327.2	478.0	224.4	105.8	50.2	24.0	11.5	5.5	2.6	1.3	0.6
0.0	1327.2	645.8	313.7	151.6	72.9	34.9	16.7	8.0	3.8	1.8	0.9
-50.0	1327.2	478.0	224.4	105.8	50.2	24.0	11.5	5.5	2.6	1.3	0.6
-100.0	10.3	11.3	13.9	10.6	6.8	4.0	2.3	1.2	0.7	0.3	0.2
MASS FLUX (mg/day)	3.00E+4	2.15E+3	1.05E+3	5.09E+2	2.47E+2	1.20E+2	5.85E+1	2.84E+1	1.38E+1	6.69E+0	3.24E+0

Target Ground water Conc, ug/L : 5.0
Modeled Area Length (L), ft : 550.0
Modeled Area Width (W), ft : 200.0
Enter Simulation Time, yr: 35

16

Displayed Model is 1st-order Decay.

Choose a Model below to Display:

Plume and Source Masses (Order-of-Magnitude Accuracy)

Plume Mass if No Biodegradation: 170.5 *kg*
- Actual Plume Mass: 9.1 *kg*
= Plume Mass Removed by Biodegradation: **161.4** *kg* (95 %)

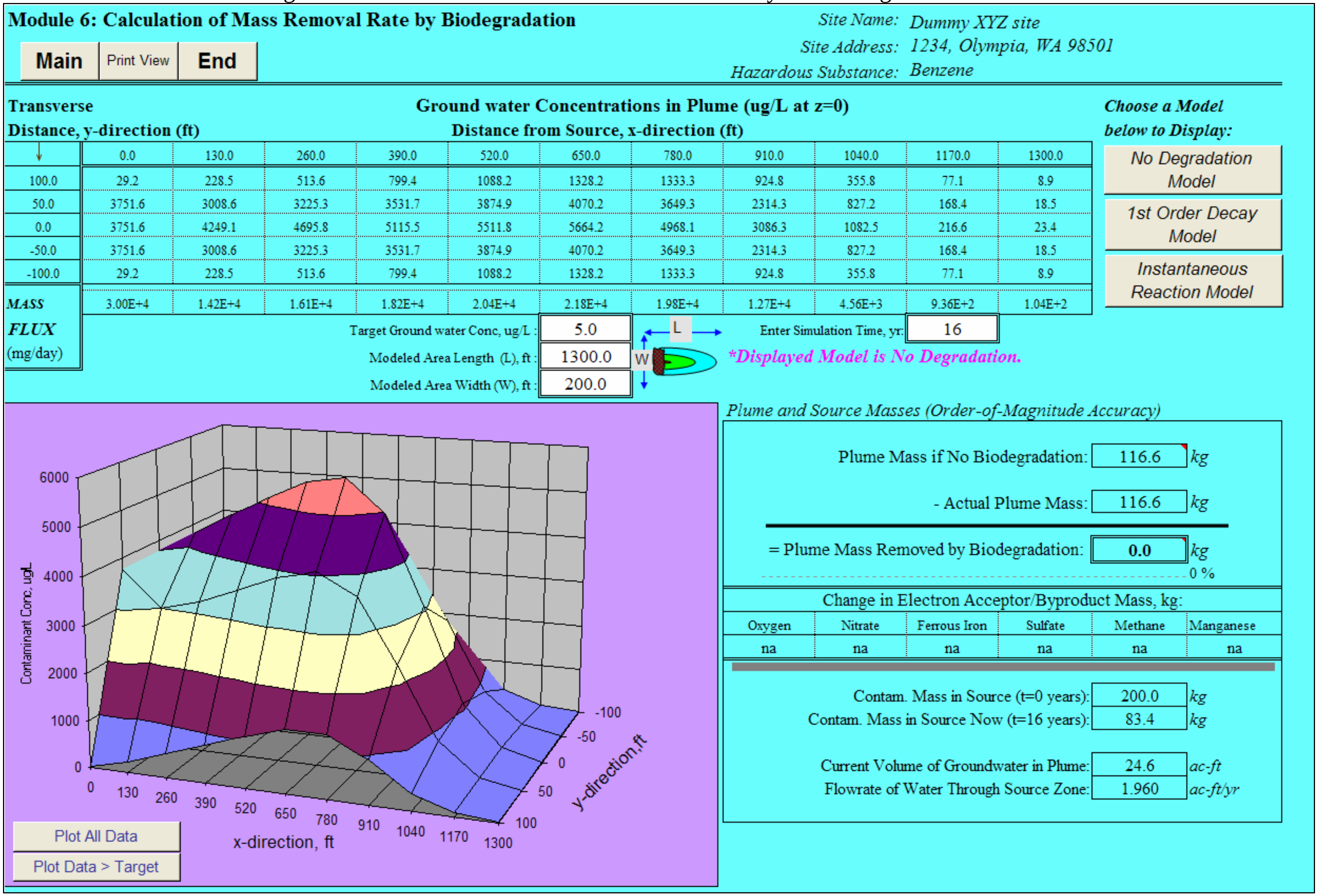
Change in Electron Acceptor/Byproduct Mass, kg:

Oxygen	Nitrate	Ferrous Iron	Sulfate	Methane	Manganese
na	na	na	na	na	na

Contam. Mass in Source (t=0 years): 200.0 *kg*
Contam. Mass in Source Now (t=35 years): 29.5 *kg*

Current Volume of Groundwater in Plume: 10.4 *ac-ft*
Flowrate of Water Through Source Zone: 1.960 *ac-ft/yr*

Figure B.6.2.c. Calculation of Mass Removal Rate by No-Biodegradation Model



Module 6: Calculation of Mass Removal Rate by Biodegradation

Site Name: *Dummy XYZ site*
Site Address: *1234, Olympia, WA 98501*
Hazardous Substance: *Benzene*

Transverse Distance, y-direction (ft)

Ground water Concentrations in Plume (ug/L at z=0)

Distance from Source, x-direction (ft)

Choose a Model below to Display:

↓	0.0	130.0	260.0	390.0	520.0	650.0	780.0	910.0	1040.0	1170.0	1300.0
100.0	29.2	228.5	513.6	799.4	1088.2	1328.2	1333.3	924.8	355.8	77.1	8.9
50.0	3751.6	3008.6	3225.3	3531.7	3874.9	4070.2	3649.3	2314.3	827.2	168.4	18.5
0.0	3751.6	4249.1	4695.8	5115.5	5511.8	5664.2	4968.1	3086.3	1082.5	216.6	23.4
-50.0	3751.6	3008.6	3225.3	3531.7	3874.9	4070.2	3649.3	2314.3	827.2	168.4	18.5
-100.0	29.2	228.5	513.6	799.4	1088.2	1328.2	1333.3	924.8	355.8	77.1	8.9
MASS FLUX (mg/day)	3.00E+4	1.42E+4	1.61E+4	1.82E+4	2.04E+4	2.18E+4	1.98E+4	1.27E+4	4.56E+3	9.36E+2	1.04E+2

Target Ground water Conc, ug/L : 5.0
Modeled Area Length (L), ft : 1300.0
Modeled Area Width (W), ft : 200.0
Enter Simulation Time, yr: 16

***Displayed Model is No Degradation.**

Plume and Source Masses (Order-of-Magnitude Accuracy)

Plume Mass if No Biodegradation: 116.6 *kg*
- Actual Plume Mass: 116.6 *kg*
= Plume Mass Removed by Biodegradation: **0.0** *kg*
0 %

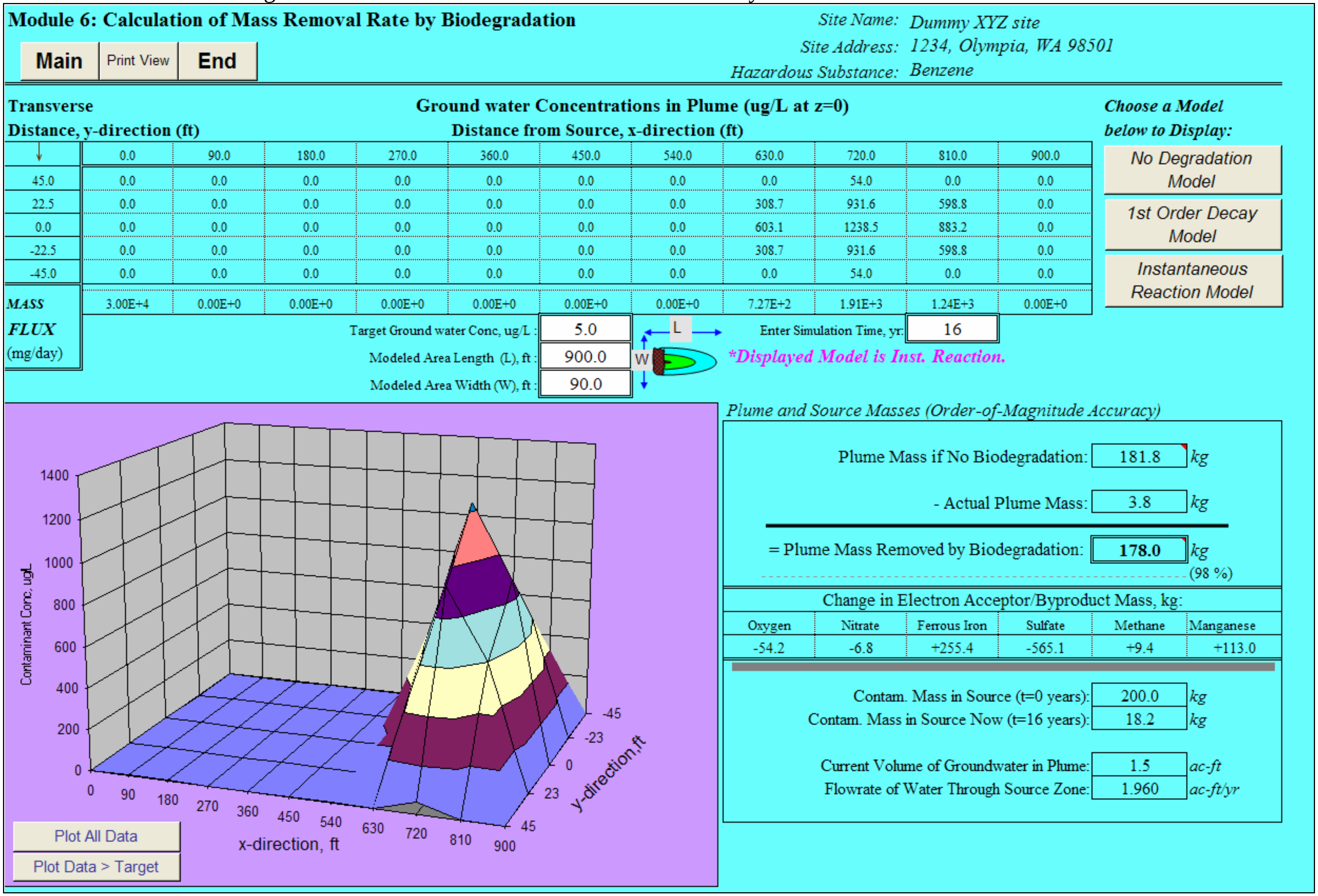
Change in Electron Acceptor/Byproduct Mass, kg:

Oxygen	Nitrate	Ferrous Iron	Sulfate	Methane	Manganese
na	na	na	na	na	na

Contam. Mass in Source (t=0 years): 200.0 *kg*
Contam. Mass in Source Now (t=16 years): 83.4 *kg*

Current Volume of Groundwater in Plume: 24.6 *ac-ft*
Flowrate of Water Through Source Zone: 1.960 *ac-ft/yr*

Figure B.6.2.d. Calculation of Mass Removal Rate by Instantaneous Reaction Model



Module 6: Calculation of Mass Removal Rate by Biodegradation

Site Name: *Dummy XYZ site*
Site Address: *1234, Olympia, WA 98501*
Hazardous Substance: *Benzene*

Ground water Concentrations in Plume (ug/L at z=0)

Transverse Distance, y-direction (ft) ↓	**Distance from Source, x-direction (ft)** 0.0	90.0	180.0	270.0	360.0	450.0	540.0	630.0	720.0	810.0	900.0
45.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	54.0	0.0	0.0
22.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	308.7	931.6	598.8	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	603.1	1238.5	883.2	0.0
-22.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	308.7	931.6	598.8	0.0
-45.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	54.0	0.0	0.0
MASS FLUX (mg/day)	3.00E+4	0.00E+0	0.00E+0	0.00E+0	0.00E+0	0.00E+0	0.00E+0	7.27E+2	1.91E+3	1.24E+3	0.00E+0

Choose a Model below to Display:

Target Ground water Conc, ug/L : 5.0
Modeled Area Length (L), ft : 900.0
Modeled Area Width (W), ft : 90.0
Enter Simulation Time, yr: 16

****Displayed Model is Inst. Reaction.***

Plume and Source Masses (Order-of-Magnitude Accuracy)

Plume Mass if No Biodegradation: 181.8 *kg*
- Actual Plume Mass: 3.8 *kg*
= Plume Mass Removed by Biodegradation: **178.0** *kg* (98 %)

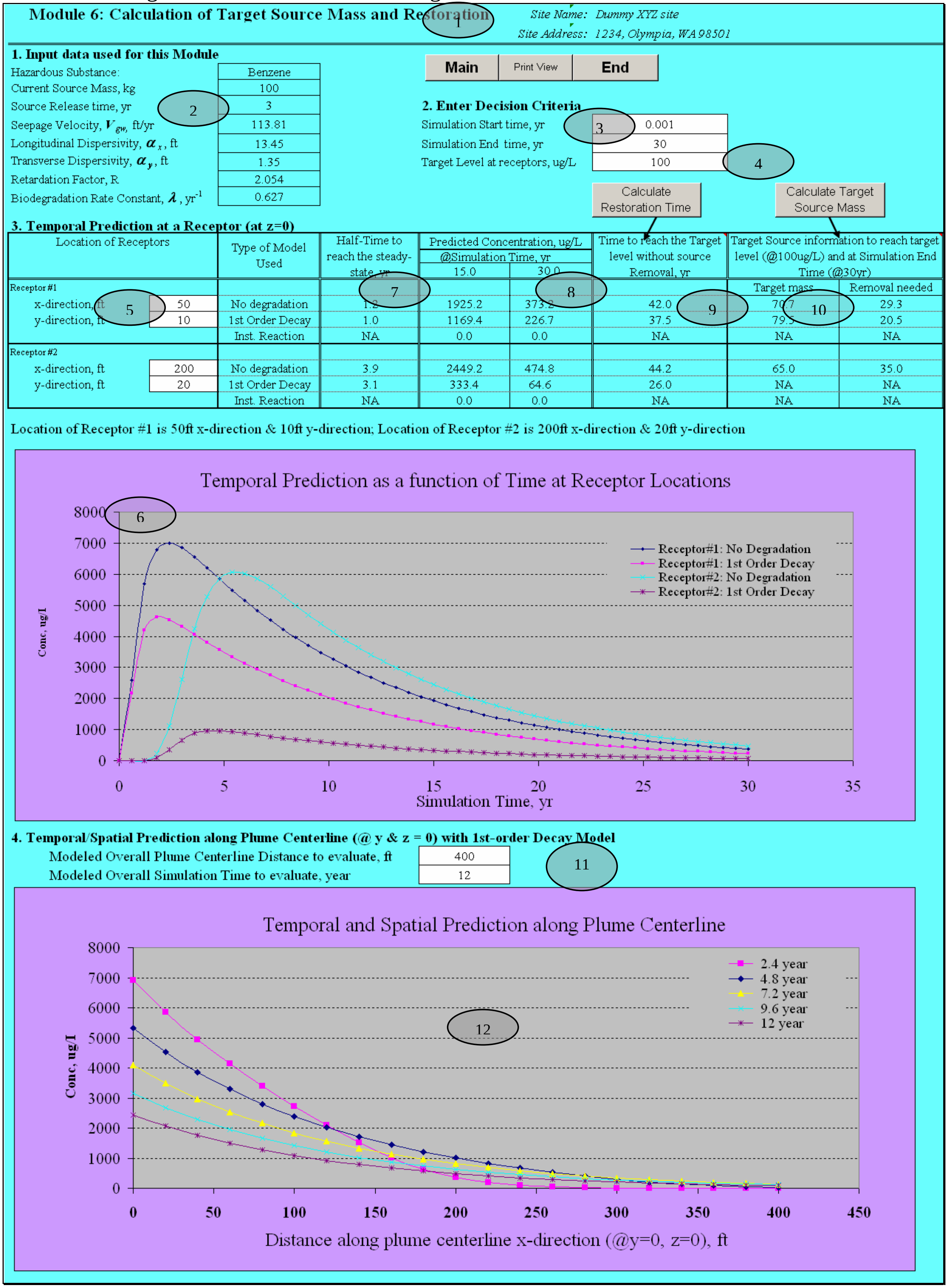
Change in Electron Acceptor/Byproduct Mass, kg:

Oxygen	Nitrate	Ferrous Iron	Sulfate	Methane	Manganese
-54.2	-6.8	+255.4	-565.1	+9.4	+113.0

Contam. Mass in Source (t=0 years): 200.0 *kg*
Contam. Mass in Source Now (t=16 years): 18.2 *kg*

Current Volume of Groundwater in Plume: 1.5 *ac-ft*
Flowrate of Water Through Source Zone: 1.960 *ac-ft/yr*

Figure B.6.3. Calculation of Target Source Mass and Restoration Time



Module 6: Calculation of Target Source Mass and Restoration

Site Name: *Dummy XYZ site*
Site Address: *1234, Olympia, WA 98501*

1. Input data used for this Module

Hazardous Substance:	Benzene
Current Source Mass, kg	100
Source Release time, yr	3
Seepage Velocity, V_{gw}, ft/yr	113.81
Longitudinal Dispersivity, α_x, ft	13.45
Transverse Dispersivity, α_y, ft	1.35
Retardation Factor, R	2.054
Biodegradation Rate Constant, λ, yr^{-1}	0.627

2. Enter Decision Criteria

Simulation Start time, yr	0.001
Simulation End time, yr	30
Target Level at receptors, ug/L	100

3. Temporal Prediction at a Receptor (at z=0)

Location of Receptors		Type of Model Used	Half-Time to reach the steady-state, yr	Predicted Concentration, ug/L @Simulation Time, yr		Time to reach the Target level without source Removal, yr	Target Source information to reach target level (@100ug/L) and at Simulation End Time (@30yr)	
				15.0	30.0		Target mass	Removal needed
Receptor #1								
x-direction, ft	50	No degradation	1.2	1925.2	373.2	42.0	70.7	29.3
y-direction, ft	10	1st Order Decay	1.0	1169.4	226.7	37.5	79.5	20.5
		Inst. Reaction	NA	0.0	0.0	NA	NA	NA
Receptor #2								
x-direction, ft	200	No degradation	3.9	2449.2	474.8	44.2	65.0	35.0
y-direction, ft	20	1st Order Decay	3.1	333.4	64.6	26.0	NA	NA
		Inst. Reaction	NA	0.0	0.0	NA	NA	NA

Location of Receptor #1 is 50ft x-direction & 10ft y-direction; Location of Receptor #2 is 200ft x-direction & 20ft y-direction

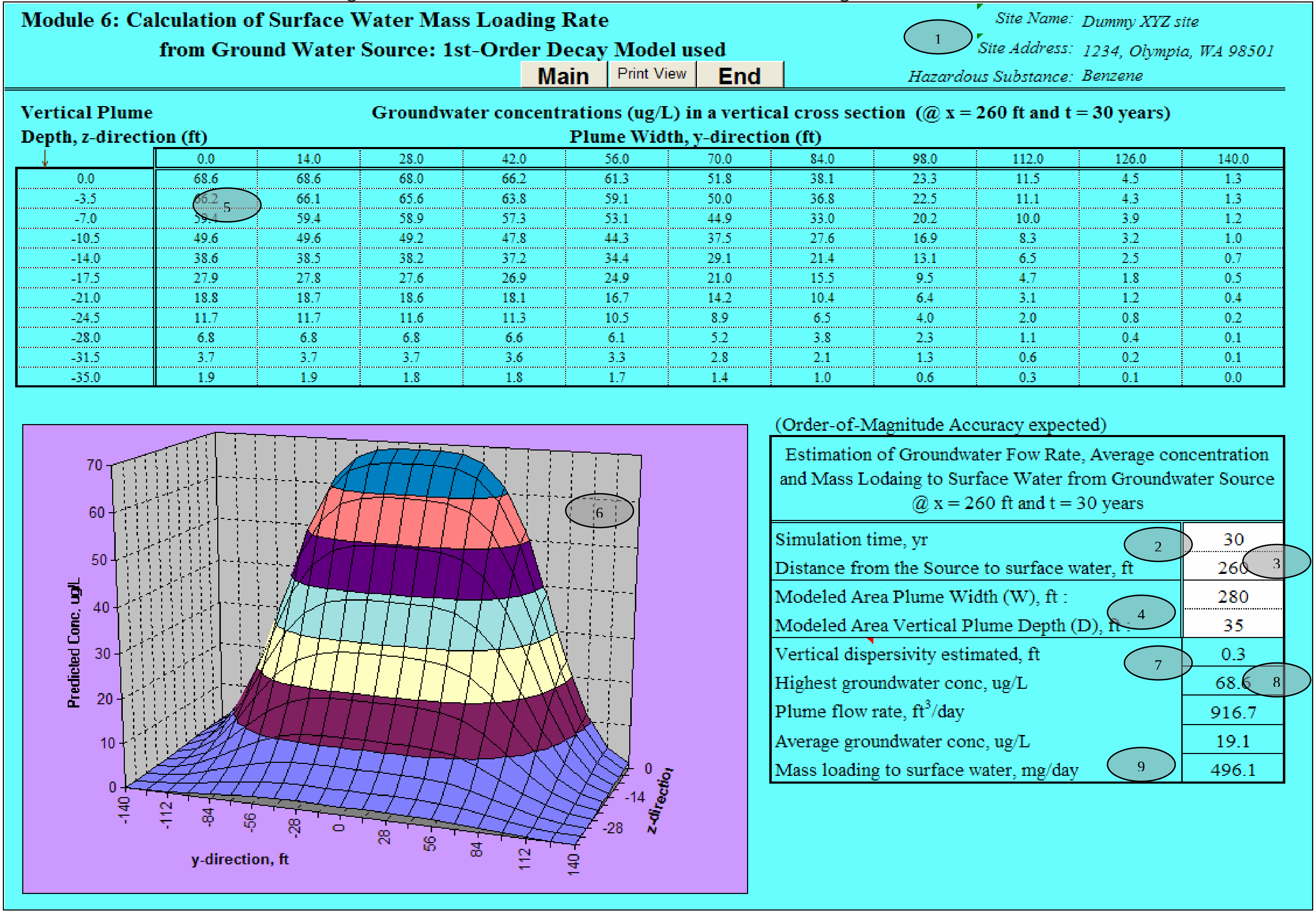
Temporal Prediction as a function of Time at Receptor Locations

4. Temporal/Spatial Prediction along Plume Centerline (@ y & z = 0) with 1st-order Decay Model

Modeled Overall Plume Centerline Distance to evaluate, ft	400
Modeled Overall Simulation Time to evaluate, year	12

Temporal and Spatial Prediction along Plume Centerline

Figure B.6.4. Calculation of Surface Water Mass Loading Rate



Module 6: Calculation of Surface Water Mass Loading Rate
from Ground Water Source: 1st-Order Decay Model used

Site Name: *Dummy XYZ site*
Site Address: *1234, Olympia, WA 98501*
Hazardous Substance: *Benzene*

Vertical Plume Depth, z-direction (ft)

Groundwater concentrations (ug/L) in a vertical cross section (@ x = 260 ft and t = 30 years)

Plume Width, y-direction (ft)

	0.0	14.0	28.0	42.0	56.0	70.0	84.0	98.0	112.0	126.0	140.0
0.0	68.6	68.6	68.0	66.2	61.3	51.8	38.1	23.3	11.5	4.5	1.3
-3.5	66.2	66.1	65.6	63.8	59.1	50.0	36.8	22.5	11.1	4.3	1.3
-7.0	59.4	59.4	58.9	57.3	53.1	44.9	33.0	20.2	10.0	3.9	1.2
-10.5	49.6	49.6	49.2	47.8	44.3	37.5	27.6	16.9	8.3	3.2	1.0
-14.0	38.6	38.5	38.2	37.2	34.4	29.1	21.4	13.1	6.5	2.5	0.7
-17.5	27.9	27.8	27.6	26.9	24.9	21.0	15.5	9.5	4.7	1.8	0.5
-21.0	18.8	18.7	18.6	18.1	16.7	14.2	10.4	6.4	3.1	1.2	0.4
-24.5	11.7	11.7	11.6	11.3	10.5	8.9	6.5	4.0	2.0	0.8	0.2
-28.0	6.8	6.8	6.8	6.6	6.1	5.2	3.8	2.3	1.1	0.4	0.1
-31.5	3.7	3.7	3.7	3.6	3.3	2.8	2.1	1.3	0.6	0.2	0.1
-35.0	1.9	1.9	1.8	1.8	1.7	1.4	1.0	0.6	0.3	0.1	0.0

(Order-of-Magnitude Accuracy expected)

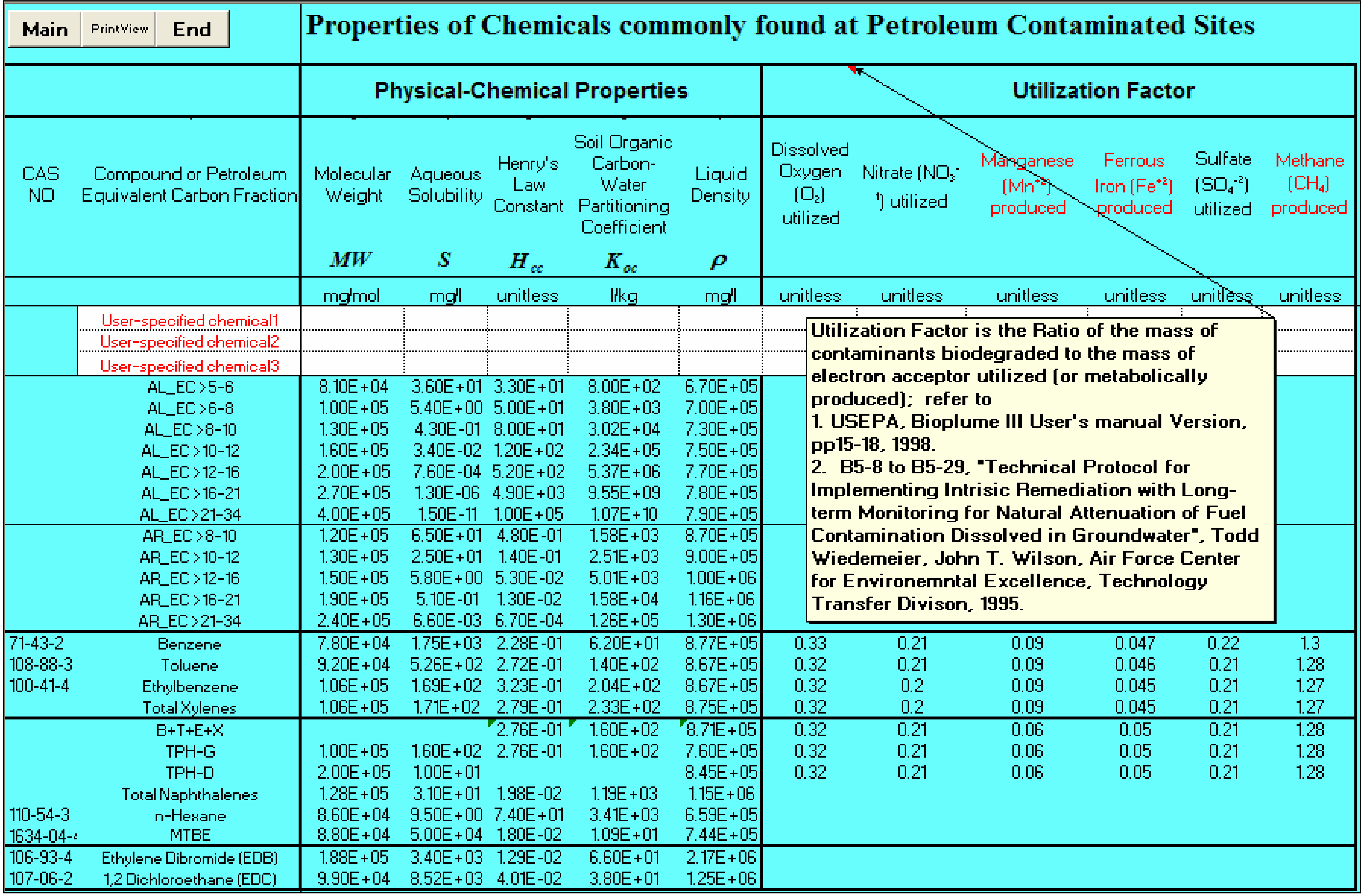
Estimation of Groundwater Fow Rate, Average concentration and Mass Lodaing to Surface Water from Groundwater Source @ x = 260 ft and t = 30 years

Simulation time, yr	30
Distance from the Source to surface water, ft	260
Modeled Area Plume Width (W), ft :	280
Modeled Area Vertical Plume Depth (D), ft :	35
Vertical dispersivity estimated, ft	0.3
Highest groundwater conc, ug/L	68.6
Plume flow rate, ft^3/day	916.7
Average groundwater conc, ug/L	19.1
Mass loading to surface water, mg/day	496.1

Appendix C

Properties of Petroleum Contaminants

Figure C.1. Data Base: Properties of Contaminants commonly found at Petroleum-Contaminated Sites



Properties of Chemicals commonly found at Petroleum Contaminated Sites

		Physical-Chemical Properties					Utilization Factor					
CAS NO	Compound or Petroleum Equivalent Carbon Fraction	Molecular Weight	Aqueous Solubility	Henry's Law Constant	Soil Organic Carbon-Water Partitioning Coefficient	Liquid Density	Dissolved Oxygen (O_2) utilized	Nitrate (NO_3^{-1}) utilized	Manganese (Mn^{+2}) produced	Ferrous Iron (Fe^{+2}) produced	Sulfate (SO_4^{-2}) utilized	Methane (CH_4) produced
		MW	S	H_{cc}	K_{oc}	ρ						
		mg/mol	mg/l	unitless	l/kg	mg/l	unitless	unitless	unitless	unitless	unitless	unitless
	User-specified chemical1											
	User-specified chemical2											
	User-specified chemical3											
	AL_EC>5-6	8.10E+04	3.60E+01	3.30E+01	8.00E+02	6.70E+05						
	AL_EC>6-8	1.00E+05	5.40E+00	5.00E+01	3.80E+03	7.00E+05						
	AL_EC>8-10	1.30E+05	4.30E-01	8.00E+01	3.02E+04	7.30E+05						
	AL_EC>10-12	1.60E+05	3.40E-02	1.20E+02	2.34E+05	7.50E+05						
	AL_EC>12-16	2.00E+05	7.60E-04	5.20E+02	5.37E+06	7.70E+05						
	AL_EC>16-21	2.70E+05	1.30E-06	4.90E+03	9.55E+09	7.80E+05						
	AL_EC>21-34	4.00E+05	1.50E-11	1.00E+05	1.07E+10	7.90E+05						
	AR_EC>8-10	1.20E+05	6.50E+01	4.80E-01	1.58E+03	8.70E+05						
	AR_EC>10-12	1.30E+05	2.50E+01	1.40E-01	2.51E+03	9.00E+05						
	AR_EC>12-16	1.50E+05	5.80E+00	5.30E-02	5.01E+03	1.00E+06						
	AR_EC>16-21	1.90E+05	5.10E-01	1.30E-02	1.58E+04	1.16E+06						
	AR_EC>21-34	2.40E+05	6.60E-03	6.70E-04	1.26E+05	1.30E+06						
71-43-2	Benzene	7.80E+04	1.75E+03	2.28E-01	6.20E+01	8.77E+05	0.33	0.21	0.09	0.047	0.22	1.3
108-88-3	Toluene	9.20E+04	5.26E+02	2.72E-01	1.40E+02	8.67E+05	0.32	0.21	0.09	0.046	0.21	1.28
100-41-4	Ethylbenzene	1.06E+05	1.69E+02	3.23E-01	2.04E+02	8.67E+05	0.32	0.2	0.09	0.045	0.21	1.27
	Total Xylenes	1.06E+05	1.71E+02	2.79E-01	2.33E+02	8.75E+05	0.32	0.2	0.09	0.045	0.21	1.27
	B+T+E+X			2.76E-01	1.60E+02	8.71E+05	0.32	0.21	0.06	0.05	0.21	1.28
	TPH-G	1.00E+05	1.60E+02	2.76E-01	1.60E+02	7.60E+05	0.32	0.21	0.06	0.05	0.21	1.28
	TPH-D	2.00E+05	1.00E+01			8.45E+05	0.32	0.21	0.06	0.05	0.21	1.28
	Total Naphthalenes	1.28E+05	3.10E+01	1.98E-02	1.19E+03	1.15E+06						
110-54-3	n-Hexane	8.60E+04	9.50E+00	7.40E+01	3.41E+03	6.59E+05						
1634-04-	MTBE	8.80E+04	5.00E+04	1.80E-02	1.09E+01	7.44E+05						
106-93-4	Ethylene Dibromide (EDB)	1.88E+05	3.40E+03	1.29E-02	6.60E+01	2.17E+06						
107-06-2	1,2 Dichloroethane (EDC)	9.90E+04	8.52E+03	4.01E-02	3.80E+01	1.25E+06						

Utilization Factor is the Ratio of the mass of contaminants biodegraded to the mass of electron acceptor utilized (or metabolically produced); refer to
1. USEPA, Bioplume III User's manual Version, pp15-18, 1998.
2. B5-8 to B5-29, "Technical Protocol for Implementing Intrisic Remediation with Long-term Monitoring for Natural Attenuation of Fuel Contamination Dissolved in Groundwater", Todd Wiedemeier, John T. Wilson, Air Force Center for Environemntal Excellence, Technology Transfer Divison, 1995.

Appendix D

Simple Fate and Transport Calculation: Natural Attenuation Processes

Definition and dimension of symbols/abbreviations used in equations shown throughout this appendix can be found in Appendix F of this guidance document (Pub. No. 05-09-091A).

D.1 Advection: Advection or a ground water seepage velocity can be calculated by:

$$v_{gw} = \frac{Ki}{n_e} \qquad \text{(Eq. D.1)}$$

Example of estimating a ground water seepage velocity and ground water travel time:
Given a hydraulic conductivity of 8 ft/day, gradient of 0.001 ft/ft, and an effective porosity of 0.35, calculate a ground water seepage velocity and elapsed time ground water will travel 800 ft.

$$v_{gw} = \frac{8\, ft/day}{0.35} * (0.001\,\mathrm{ft/ft}) = 0.023\,\mathrm{ft/day}$$

Travel time can then be estimated to be:

$$t = \frac{x}{v_{gw}} = \frac{800\ ft}{0.023\ ft/day} * \frac{year}{365\,day} = 96\,year$$

D.2 Biodegradation (1st-Order): Biodegradation by 1st- order decay can be calculated by:

$$C_t = C_{start} * \exp\left(-k_{po\,\mathrm{int}}\,t\right) \qquad \text{(Eq. D.2)}$$

Example of estimating biodegradation by 1st-order decay:
Given a benzene concentration in ground water of 5 mg/L, estimate the remaining concentrations after 3 years for 1% per day decay rate.

$$C_t = C_{start} * \exp\left(-k_{po\,\mathrm{int}}\,t\right) = 5{,}000\,\mu g/L * \exp(-0.01/day * 3 * 365 day) = 0.088\,\mu g/L$$

D.3 Dispersion: There are two components of dispersion; mechanical mixing, and molecular diffusion. Since molecular diffusion is very rarely observed on a field scale, the following example will be only for mechanical dispersion (Eq. D.3), which is defined as:

$$Dispersion\ (Mechanical\ Mixing\ ) = \alpha v_{gw} \qquad \text{(Eq. D.3)}$$

There are three components to dispersion: α_x, or longitudinal, in the main direction of ground water flow; α_y, or transverse, perpendicular to the main direction of ground water flow; and α_z, or vertical, which is perpendicular in the “Z” direction to the main component of flow. Transverse (α_y) is generally less than longitudinal (α_x) and vertical (α_z) is usually significantly less than α_y. The one-dimensional advection – dispersion equation is given by:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v_{gw} \frac{\partial C}{\partial x} \qquad \text{(Eq. D.4)}$$

Bear (1961) allows for the advection-dispersion equation (Eq. D.5) for the continuous source to be solved by:

$$C_{x,t} = \left(\frac{C_0}{2}\right) * \left\{ erfc\left[\frac{x - v_{gw}t}{2\sqrt{(D_x t)}}\right] + \exp\left(\frac{v_{gw}x}{D_x}\right) * erfc\left[\frac{x + v_{gw}t}{2\sqrt{(D_x t)}}\right]\right\} \qquad \text{(Eq. D.5)}$$

where "erfc" is the complementary error function which can be found in ground water text books that address ground water flow and transport. Note that the second term can be neglected for most practical problems.

Example of Dispersion:
Estimate the time it will take for benzene concentrations to reach 100 μg/L at 750 feet from the source. Assume K = 86.4 ft/day, $n_e = 0.2$, $i = 0.002$ ft/ft, C_o = 1,000 μg/L, α_x = 75 ft, one dimensional flow, ignoring biodegradation and sorption.

Step 1 – Calculate seepage velocity:

$$v_{gw} = \frac{Ki}{n_e} = \frac{86.4\, ft/day * 0.002\, ft/\, ft}{0.2} = 0.86\, ft/day$$

Step 2 – Calculate dispersion:

$$D_x = \alpha_x v_{gw} = 75\, ft * 0.86\, ft/day = 64.8\, ft^2/day$$

Step 3 – Using equation (Eq. D.5) above (ignore 2nd term) and solving for time:

$$C_{x,t} = \frac{C_0}{2} * erfc\left(\frac{x - v_{gw}t}{2\sqrt{(D_x t)}}\right) =$$

$$100 = \frac{1000}{2} * erfc\left(\frac{750 - 0.86t}{2\sqrt{64.8t}}\right)$$

With trial and error or Microsoft EXCEL^{TM} built-in "SOLVER" function,

t = 495 day

D.4 Retardation: Retardation is calculated from the soil organic carbon-water partitioning coefficient (K_{oc}) for sorption as:

$$R = 1 + \frac{K_{oc} f_{oc} \rho_b}{n_e} \qquad \text{(Eq. D.6)}$$

Retarded transport velocity of contaminant can be calculated by:

$$v_c = \frac{v_{gw}}{R} \qquad \text{(Eq. D.7)}$$

Example of Retardation:
Calculate the retarded contaminant velocity for benzene assuming fraction organic carbon (f_{oc}) = 0.5%, hydraulic gradient of 0.001 ft/ft, hydraulic conductivity of 10 ft/day, effective porosity of 0.3, and bulk density of 1.58 g/ml, K_{oc} = 78 ml/g.

Step 1 – calculate ground water seepage velocity:

$$V_{gw} = \frac{10\, ft/day * 0.001\, ft/\, ft}{0.3} = 0.033\, ft/day$$

Step 2 – calculate retardation factor:

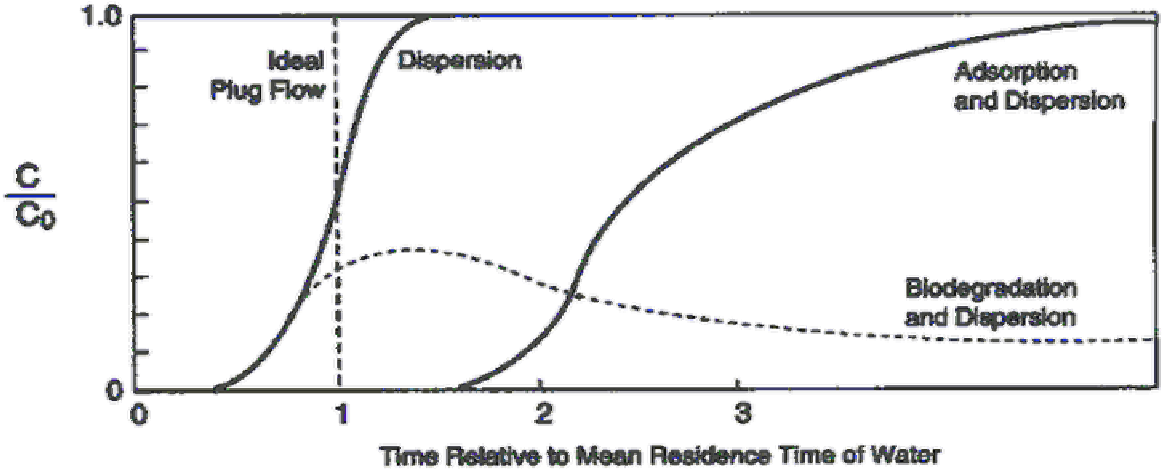
$$R = 1 + \frac{78 ml/g * 0.005 * 1.58 g/ml}{0.3} = 3.05$$

Step 3 – calculate contaminant velocity:

$$v_c = \frac{v_{gw}}{R} = \frac{0.033\, ft/day}{3.05} = 0.011\, ft/day$$

Figure D.1 illustrates the effect of natural attenuation mechanisms that include advection, dispersion, adsorption, and biodegradation on the concentration of contaminants in ground water. Dispersion causes contaminants to spread. Adsorption and biodegradation cause concentration to decrease. In considering the average ground water flow velocity, contaminant travel time is significantly underestimated (Hal White, US EPA/OUST, Personal Communication, 2004). As shown in Figure D.1, due to dispersion, approximately half the mass of the plume arrives before an ideal slug of contamination (represented by the average velocity) and approximately half arrives later. Looking down at the x-axis, the time of first arrival occurs in approximately half the time that the ideal slug is traveling at the average velocity. In order to ensure protectiveness, it would be more prudent to use the maximum contaminant transport velocity rather than the average rate.

Figure D.1. Effects of Dispersion, Adsorption, and Biodegradation on the Contaminant Concentration in Ground Water



Adapted from NRC (2000)

Appendix E

Example Problem

This sample report presents the result of a feasibility study performed by a consultant at ABC store in Olympia, WA to evaluate the use of natural attenuation with long-term monitoring as a cleanup action for dissolved phase BTEX contamination in the shallow ground water.

E.1 Site Background

The site, ABC store, is located in Olympia, WA, and is an active retail petroleum service station. The properties surrounding the site are mixed residential and industrial. No public or private wells or surface water body exist within a ½ mile radius of the site, and city ordinances require a hookup to the municipal water supply. Any potential ground water exposure pathway was examined including soil vapor migration, surface water bodies, supply wells, and any nearby sensitive ecosystems such as threatened or endangered species within the three-year travel time of ground water and within a ½ mile radius of the site. No potential exposure pathway will be complete under future land or ground water use assumptions provided use of ground water as a potable source of water is prohibited by institutional controls within and down-gradient of the source area.

No change in land or ground water use is anticipated in the foreseeable future. Shallow ground water is not used to meet the domestic potable water demands at the subject site. The site was found to have relatively simple and well understood hydrogelogy (single layer unconsolidated ground water-bearing unit). Hydrogeologic conditions of the subject property do not appear to change greatly over time (i.e. no significant change in the direction of ground water flow or velocity). The levels of MTBE concentration in the ground water source zone and plume are minimal. Ground water does not likely discharge at the ground surface or into a surface water body.

During a service station upgrade conducted in 1991, subsurface petroleum hydrocarbon impacts were noted in the vicinity of the dispenser islands. The date of the release is unknown. Subsequently, ten monitoring/observation wells were installed on site (Figure E.1). Four tank pit monitoring wells were installed but cannot be used for the natural attenuation evaluation since they were not sampled after 1992. Free product was first encountered at MW-2 in February 1992 with a thickness of 1/8 inch which increased to 5/8 inch in May 1992. Ground water flow is to the northwest, as shown in Figure E.1.

An initial investigation of the site was performed by the Washington State Department of Ecology. A thorough site characterization and a remedial investigation and feasibility study conducted in accordance with WAC 173-340-350 were completed by the owner of ABC store. Interim Soil Vapor Extraction (SVE) and product recovery activities were completed by the owner in 1993. As a result, soil contamination was reduced to below the remediation standards, but the ground water does not meet cleanup levels at the point of compliance. Representative ground water isopleth concentrations for benzene are shown on Figure E.2.

Since no current threat to existing/potential receptors was identified from site conditions, effective source control was achieved, no product was detected in site monitoring wells after May 1992, and soil concentrations met remediation standards, it was judged that this site may be suitable for remediation by natural attenuation as suggested by an Ecology site manager. Both Ecology and the liable party agreed that source control had been conducted to the maximum extent practicable. The wells selected to determine if natural attenuation was occurring and will continue to occur at a reasonable rate at the subject site and within the plume included MW-1, MW4, MW6, MW7 and MW-8, as shown on Figure E.2.

E.2 Natural Attenuation Evaluation

In order to demonstrate the effectiveness of natural attenuation as a cleanup action, the plume status needs to be determined (expanding, stable, or shrinking). The data for ABC store were evaluated using Modules 1, 2, and 3 of the "Natural Attenuation Analysis Tool Package A" as illustrated below.

Module 1: Non-Parametric Analysis for Plume Stability Test:

Data for MW-1 for benzene, toluene, ethylbenzene, total xylenes, and MTBE were entered from 1996 to 2000 (16 or fewer sampling events). For demonstration purposes, MW-1 has been selected since it is in the area of highest impact. Historical contaminant concentrations data from other wells should also be analyzed using this method. The following summarizes the results of Module 1 for MW-1:

<u>Mann-Kendall Test Worksheet</u> (Figure E.3)
- Data from 1996 to 2000 were used in this analysis.
- With the 85% confidence level used as a decision criterion, the Mann-Kendall quantitative trend analysis for all five contaminants indicates that the plume is "Shrinking" at MW-1.
- The Mann-Kendall statistic "S" value is substantially less than "zero" for all five contaminants, which indicates a decreasing concentration trend at MW-1.
- The trend graphs show a pronounced downward trend in concentration for each contaminant in all monitoring wells selected.

Similar results were obtained for all other monitoring wells at the site with sufficient data to conduct the analysis. In addition, no contaminants were detected at a sentinel well (MW-8) located at the leading edge of the contaminant plume during a 10-year monitoring period.

SUMMARY OF MODULE 1: Based on the above analysis and the guidance in Table 3.2 of Ecology Pub. No. 05-09-091, it can be concluded that overall site PLUME STATUS is shrinking.

Module 2: Graphical and Regression Analysis for Plume Stability and Restoration Time Calculation:

Since Module 1 established that the plume is shrinking, the focus of Module 2 will be to develop restoration time frames based on rate constants estimated for the overall plume. The data are entered into Module 2 by first entering the information into the worksheet of "Historical Ground water Data Entry". Information in this module allows for a visual evaluation of the plume status. Module 2 also allows calculation of a point decay rate constant, $k_{po\int}$ and evaluation of the relationship between ground water elevations and ground water concentrations. The following summarizes the results of Module 2 evaluation.

Historical Ground Water Data Entry Worksheet (Figure E.4)

- A hydraulic flow path across the site was derived to illustrate the change in contaminant concentrations as ground water flows from the source area. See Figure E.1.
- Concentrations for benzene from 16 sampling rounds for the sequence of monitoring wells MW-1, MW-7, MW-6, MW-4, and MW-8 were entered into the worksheet. Also, ground water elevations were entered for each of the monitoring wells to assess the impact of ground water elevation fluctuation on benzene concentration at each well. Refer to Figure E.4.

Temporal (well-to-well) Analysis Worksheet (Figure E.5)

- The restoration time for benzene (when the cleanup level of 5.0 µg/L has been entered) for all monitoring wells is estimated to average between 2 and 11 years. With 85% confidence level, the estimated time to reach the cleanup criterion ranges from 2 to 15 years from the date of the first sampling event entered into this module (5/28/96). It is important to evaluate the model predictions vs. actual analytical data to be able to calibrate the model prediction with actual site conditions. Based on this calibration of the data using the average concentration predicted at each well, an estimated restoration time frame for the site would be 2007 (or 2011 with 85% confidence level), and a performance monitoring program should be developed based on this date. Ecology agreed that the restoration time frame estimated is reasonable.
- As shown on Figure E.4, ground water data for MW-4 and MW-8 were not always collected due to consistently low levels of contaminant concentrations. Therefore, on the worksheet outputs of Figure E.5, it shows that calculation of a decay rate and determination of the plume status at these wells are not necessary. The data from MW1, MW-7, MW-4, and MW-6, however, clearly support that natural attenuation is occurring and the plume is shrinking.

Graphical Presentation of Historical Ground Water Data Worksheet (Figure E.6)

- The confidence limit for the regression graph on temporal trends at all monitoring wells for benzene is well above the 85% confidence level, which clearly indicates an overall shrinking trend. The $k_{po\mathrm{int}}$ value for calculating temporal trends is also computed along with a lower boundary estimate for $k_{po\mathrm{int}}$ at the 85% confidence level limit.
- The corresponding log-linear regression graph of benzene concentration vs. time at MW-1 displayed in the worksheet indicates a decreasing log-linear trend for benzene concentration.
- The log-linear regression graph of benzene concentration vs. ground water elevation at MW-1 and other wells shows little or no correlation between the benzene concentration and ground water elevations at any monitoring well. This suggests that the trend is real and independent of ground water elevation fluctuations.
- Evaluation of spatial and temporal trends along the overall plume length for multiple wells was not very feasible. The reasons were that the plume centerline was not identified clearly due to the relatively short overall plume length, and the congested nature of the overall plume.

SUMMARY OF MODULE 2: Overall site PLUME STATUS is shrinking, natural attenuation is occurring at the site, and the restoration time frame is determined to be acceptable based on the factors described in Section 3.2.1 of the guidance document (Pub. No. 05-09-091).

Module 3: Expressed Assimilative Capacity Calculation and Geochemical Indicator Evaluation:

Under WAC 173-340-370(7), in order for natural attenuation to be acceptable as a cleanup action, there needs to be evidence that natural biodegradation or chemical degradation is occurring at a reasonable rate at the site. Module 2, described above, established that natural attenuation at the example site will occur at a reasonable rate. Module 3 can be used to support that biodegradation is occurring by evaluating the geochemical indicators. Data from the background well are important to include in this evaluation as baseline information. For analysis purposes, the geochemical indicator data from MW-5 are used as the background. The following presents the results of Module 3:

Expressed Assimilative Capacity Calculation (Figure E.7)
The expressed assimilative capacity indicates that the site demonstrates the ability to biodegrade the hazardous substances, supporting that biodegradation is occurring at the site.

Geochemical Indicator Plot and Evaluation (Figure E.7)
The inverse relationship between dissolved oxygen (and nitrate) and benzene supports that biodegradation is occurring at the site.

SUMMARY OF MODULE 3: There is strong and clear evidence that natural biodegradation is occurring.

E.3 Summary of Feasibility Study on Natural Attenuation as a Cleanup Action Alternative

Based on the results of Modules 1, 2, and 3 calculations, natural attenuation (including biodegradation) is occurring at the site. Natural attenuation alone will achieve cleanup standards without posing an unacceptable threat to human health and the environment within a reasonable restoration time frame. Historical dissolved BTEX data from 1996 to 2000 show that the extent of dissolved BTEX contamination has remained steady and shrinking, and that down-gradient migration of dissolved contamination has not occurred.

Analysis of field data suggests that degradation of BTEX through aerobic respiration, nitrate reduction, sulfate reduction, iron reduction, manganese reduction, and methanogenesis also is occurring at the site. Sulfate reduction has been observed to dominate biodegradation processes, suggesting that ground water throughout the region favors sulfate reduction over other biodegradation reactions.

Long-term performance ground water monitoring will continue to verify the effects of natural attenuation and help predict the effects of natural attenuation. Natural biodegradation of dissolved petroleum hydrocarbons is occurring and will prevent the migration of the dissolved BTEX plume. More comprehensive fate and transport models contained in Modules 5 and 6 do not seem to be necessary for the example site.

Figure E. 1. Location of Monitoring Wells

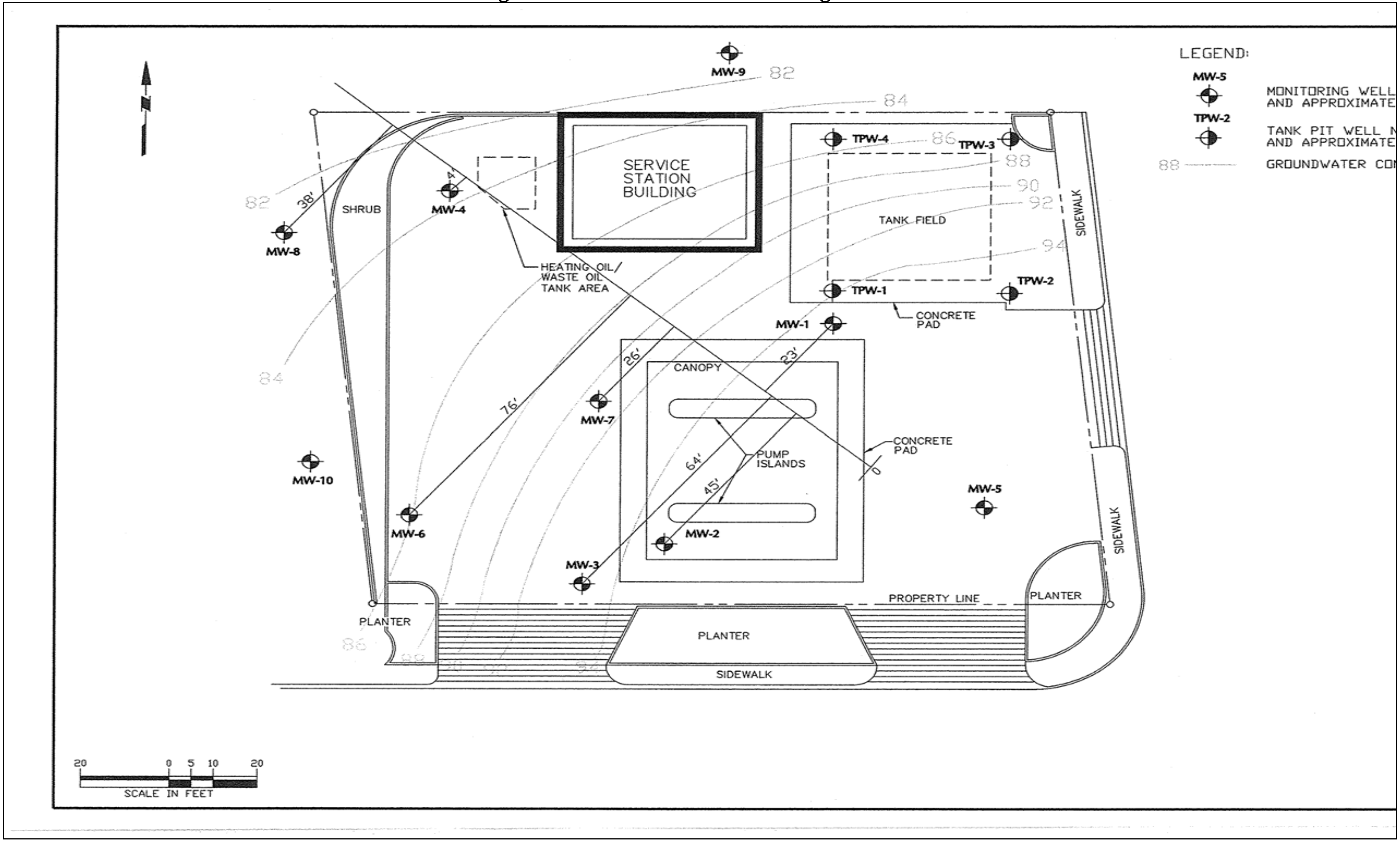


Figure E. 2. Plume Contours

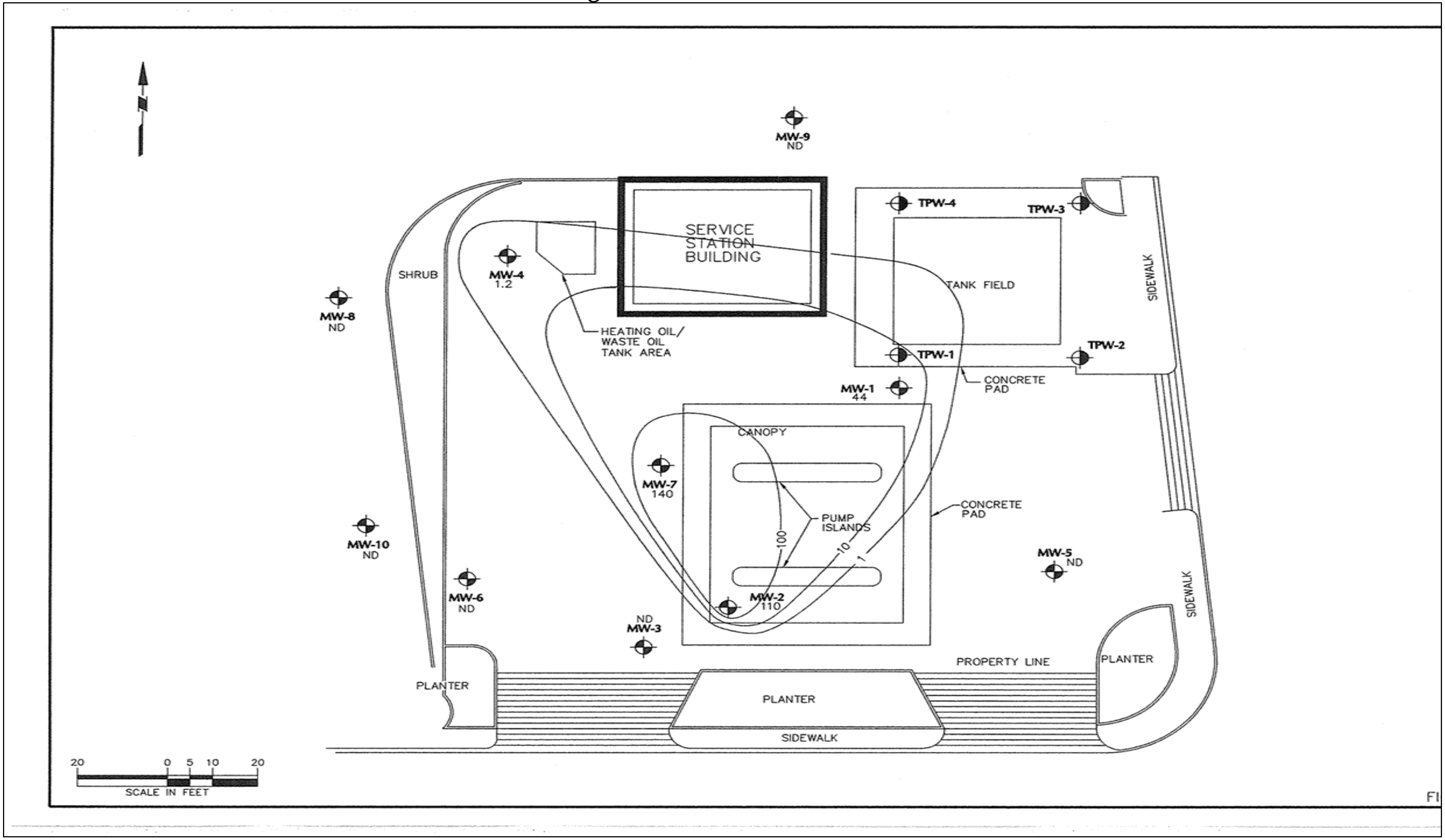


Figure E. 3. Mann-Kendall Trend Test

Module1: Mann-Kendall Trend Test for Plume Stability (Non-parametric Statistical Test)

Site Name: *ABC Store*
Site Address: *Olympia, WA*
Additional Description: *Demo NA site*

Well (Sampling) Location? **MW-1**
Level of Confidence (Decision Criteria)? **85%**

1. Monitoring Well Information: Contaminant Concentration at a well: Quarterly sampling recommended.

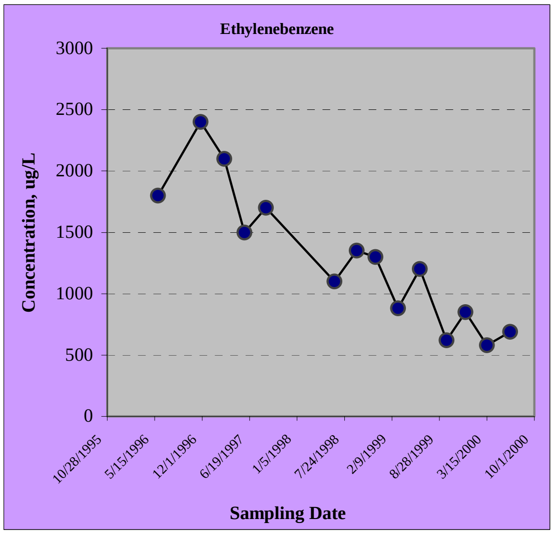
		Hazardous Substances (unit is ug/L)					
Sampling Event	Date Sampled	Benzene	Toluene	Ethylenebenzene	Xylenes	MTBE	
#1	5/28/1996	4500	700	1800	14000		
#2	6/27/1996	6700	110			25	
#3	11/25/1996	2300	33	2400	15000	12	
#4	3/4/1997		190	2100	9000		
#5	5/28/1997	956	71	1500		10	
#6	8/26/1997	270		1700	14000	50	
#7	2/17/1998		25		9200	30	
#8	6/11/1998	340	35	1100		380	
#9	9/14/1998	44	23	1350	8000	3	
#10	12/1/1998	94	25	1300	2800	5	
#11	3/6/1999	32	18	880	4900	5	
#12	6/6/1999	21	21	1200	3400	5	
#13	9/27/1999	21	19	620	1800	5	
#14	12/16/1999	45	16	850		5	
#15	3/15/2000	22	20	580	1900	5	
#16	6/21/2000	48	11	690	1100	4	

2. Mann-Kendall Non-paramteric Statistical Test Results

Hazardous Substance?	**Benzene**	**Toluene**	**Ethylenebenzene**	**Xylenes**	**MTBE**	
Confidence Level Calculated?	100.00%	100.00%	100.00%	100.00%	98.20%	NA
Plume Stability?	Shrinking	Shrinking	Shrinking	Shrinking	Shrinking	NA
Coefficient of Variation?						n<4
Mann-Kendall Statistic "S" value?	-60	-82	-71	-53	-40	0
Number of Sampling Rounds?	14	15	14	12	14	0
Average Concentration?	1099.50	87.80	1290.71	7091.67	38.86	NA
Standard Deviation?	2049.87	175.99	560.43	5175.20	99.11	NA
Coefficient of Variation?	1.86	2.00	0.43	0.73	2.55	NA
Blank if No Errors found						n<4

3. Temporal Trend: Plot of Concentration vs. Sampling Time

Hazardous substance? **Ethylenebenzene**
Plume Stability? **Shrinking**



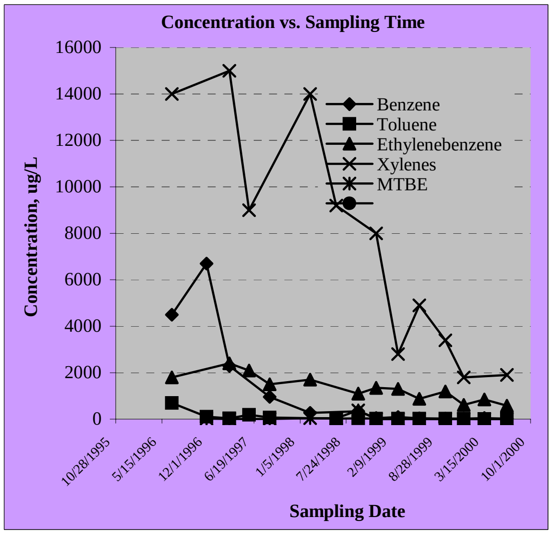


Figure E. 4. Inputs for Regression Analysis

Module 2: Inputs: Enter Historical Ground Water Data

Site Name:	*ABC Store, Olympia, WA*
Site Address:	*1234 Olymmpia, WA 98504*
Additional Description:	*Example site*
Hazardous Substance	*Benzene*

1. Monitoring Well information: Contaminant Concentration at a well:

Well Location:		Unit	MW-1	MW-7	MW-6	MW-4	MW8	MW6
Dist from source, x-direction		ft	0.001	26	40	90	110	
Off-centerline dist, y-direction		ft	0.001	0	76	4	38	
Sampling Event	Date sampled	day	Unit of concentration is ug/L					
#1	5/28/96	0	4500	1400	14	5	0.3	
#2	6/27/96	30	6700	640	7.2	3	0.3	
#3	11/25/96	181	2300	2200	2	2.4	0.3	
#4	3/4/97	280		1300	16	0.3	0.3	
#5	5/28/97	365	956	1200	33	0.3		
#6	8/26/97	455	270	790	22			
#7	2/17/98	630		1200	12			
#8	6/11/98	744	340	760	4.5			
#9	9/14/98	839	44	140	0.3	1.2	0.3	
#10	12/1/98	917	94	960				
#11	3/6/99	1012	32	870	2.5	0.9	0.3	
#12	6/6/99	1104	21	440				
#13	9/27/99	1217	21	150	0.5	0.6	0.3	
#14	12/16/99	1297	45	260	0.5	0.6		
#15	3/15/00	1387	22	430			0.3	
#16	6/21/00	1485	48	70	0.3	0.3		
#17								
#18								
#19								
#20								
Average Concentration			1099.5	800.6	8.8	1.5	0.3	N/A
Maximum Concentration			6700	2200	33	5	0.3	NA
Minimum Concentration			21	70	0.3	0.3	0.3	NA

2. Groundwater Elevation:

Well Location:			MW-1	MW-7	MW-6	MW-4	MW8	MW6
Sampling Event	Date sampled	Day	Unit of elevation is feet.					
#1	5/28/96	0	96.12	92.41	85.71	84.17	82.78	
#2	6/27/96	30	94.88	91.34	84.88	83.3	81.95	
#3	11/25/96	181	95.79	92.2	85.24	83.65	82.41	
#4	3/4/97	280	96.02	92.22	85.45		82.49	
#5	5/28/97	365	95.92	92.23	85.58		82.49	
#6	8/26/97	455	95.13	91.39	85.04		82.05	
#7	2/17/98	630	95.88	92.25	85.25		81.6	
#8	6/11/98	744	95.73	91.92	85.18		82.03	
#9	9/14/98	839	94.51	91.09	84.57		82.54	
#10	12/1/98	917	94.99	91.85	84.82		82.25	
#11	3/6/99	1012	95.99	92.42	85.43		81.85	
#12	6/6/99	1104	95.8	92.02	85.32		82.11	
#13	9/27/99	1217	95.7	92.8	85.66		82.89	

Figure E. 5. Temporal Regression Analysis

Module 2: Temporal Analysis: Concentration of contaminant vs. time (Regressi

Site Name: *ABC Store, Olympia, WA*
Site Address: *1234 Olymmpia, WA 98504*
Additional Description: *Example site*
Hazardous Substance *Benzene*

1. Level of Confidence (Decision Criteria)? **85%**

2. Prediction: Calculation of Restoration Time and Predicted Concentration at Wells

Well Location		**MW-1**	**MW-7**	**MW-6**	**MW-4**
A. Cleanup Level (Criterion) to be achieved?	ug/L	5	5	5	5
A.1 Average (@50% CL^1 best-fitting values)					
Time to reach the criterion	yr	4.67	10.99	1.39	-2.66
Date when the Criterion to be achieved	date	1/28/01	5/23/07	10/16/97	9/30/93
A.2 Boundary (@85% CL)					
Time to reach the criterion^2	yr	5.30	14.98	1.92	-6.00
Date when the Criterion to be achieved	date	9/15/01	5/17/11	4/29/98	5/30/90
B Date of Prediction?	date	5/16/09	1/1/05	1/1/05	1/1/05
B.1 Average conc predicted (@50% CL)	ug/L	0.00	17.74	0.00	0.07
B.2 Boundary conc predicted (@85% CL)	ug/L	0.00	59.66	0.05	0.43

3. Log-Linear Regression Results

Coefficient of Determination	r^2	0.873	0.538	0.580	0.328
Correlation Coefficient	r	-0.934	-0.733	-0.761	-0.573
Number of data points	n	14	16	13	10

4. Statistical Inference on the Slope of the Log-Linear Regression Line with t-statistics

One-tailed Confidence Level calculated, %	100.000%	99.877%	99.751%	91.635%
Sufficient evidence to support that the slope of the regression line is significantly different from zero?	YES!	YES!	YES!	YES!
Coefficient of Variation?	NA	NA	NA	NA
Plume Stability?	Shrinking	Shrinking	Shrinking	Shrinking

5. Calculation of Point Decay Rate Constant (k_{point})

Slope: Point decay rate constant (k_{point})	@50% CL	yr^{-1}	1.402	0.530	0.963	0.380
	@85% CL	yr^{-1}	1.235	0.389	0.696	0.168
Half Life for (k_{point})	@50% CL	yr	0.494	1.308	0.719	1.826
	@85% CL	yr	0.561	1.783	0.997	4.120

Note: 1. CL : Confidence Level; UD= Undetermined

2. The length of time that will actually be required is estimated to be no than years calculated (@ 85% of confidence level.)

Figure E. 6. Graphical Presentation of Temporal Trend

Module 2: Graphical Presentation of Historical Ground Water Data: (Well to Well Analysis)

Site Name: *ABC Store, Olympia, WA*
Site Address: *1234 Olymmpia, WA 98504*
Additional Description: *Example site*
Hazardous Substance *Benzene*

1. Temporal Trend at a Well (Concentration vs. Time & Groundwater Elevation : well-to-well analysis)

Name of Sampling Well?	**MW-1**	Confidence Level (Decision Criteria)?	85.0%		
Confidence Level calculated with log-linear regression is?	*100.000%*				
Plume Stability?	Shrinking	; Decision Criteria is 85%.			
Slope: Point decay rate constant ($\boldsymbol{k}_{point}$), yr^{-1}	*1.402*	@50% C.L.;	*1.235*	@85% C.L.	
Half Life for $\boldsymbol{k}_{point}$, yr	*0.494*	@50% C.L.;	*0.561*	@85% C.L.	

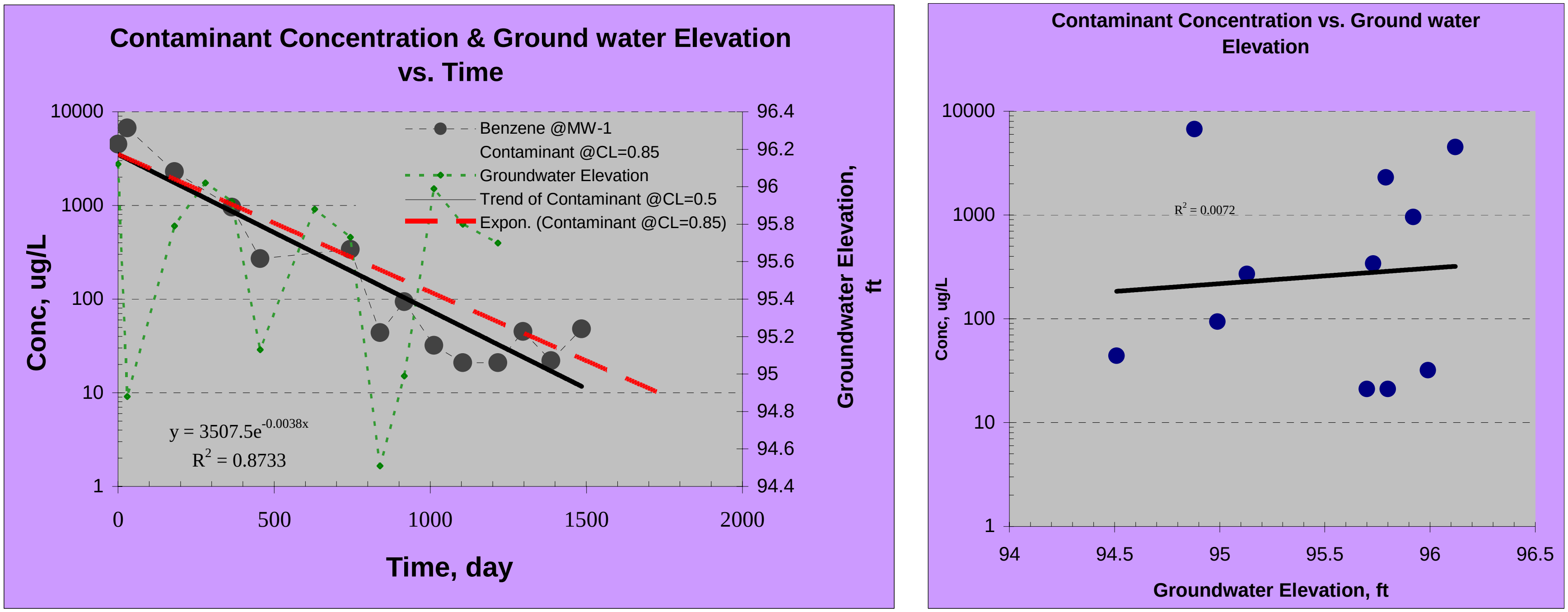


Figure E.7. Analysis of Geochemical Indicators

Module 3: Assimilative Capacity Calculation and Geochemical Indicator Plot

Site Name: *ABC store, Olympia, WA*
Site Address: *1234, olympia, WA 98504*
Additional Description: *Demo NA site*

1. Monitoring Well information: Average Contaminant Concentrations at the Monitoring Wells

Sampling Location:	Unit				MW-5	Mw-1	Mw-7	Mw-6						
Centerline Distance from source	ft				-50	0	26	40						
Benzene	ug/L				0.3	1100	800	8.8						
Toluene	ug/L				0.5	87.8	44	5.5						
Ethylbenzene	ug/L				0.5	1290	325	56						
Total Xylenes	ug/L				0.5	7091	1230	125						
BTEX	ug/L													
User-specified chemical2	ug/L													
User-specified chemical3	ug/L													

2. Average Geochemical Indicator's Concentrations at the Monitoring Wells.

		Unit	Background	NA	NA	MW-5	Mw-1	Mw-7	Mw-6	NA	NA	NA	NA	NA	NA
Dissolved Oxygen	utilized	mg/L	**4.5**			4.5	0.2	1.2	2.5						
Nitrate	utilized	mg/L	**35**			35	0.6	0.6	2						
Sulfate	utilized	mg/L	**65**			65	7.8	45	67						
Manganese	produced	mg/L	**1.2**			1.2	23.3	9.5	4.5						
Ferrous Iron	produced	mg/L	**2.5**			2.5	89.5	45	25						
Methane	produced	mg/L	**0.5**			0.5	8.5	5.6	4.7						
Redex Potential	Change	mV													
Alkalinity	Change	mg/L													
pH	change	unitless													

3. Expressed Assimilative Capacity Calculation: Utilization Factor (UF)

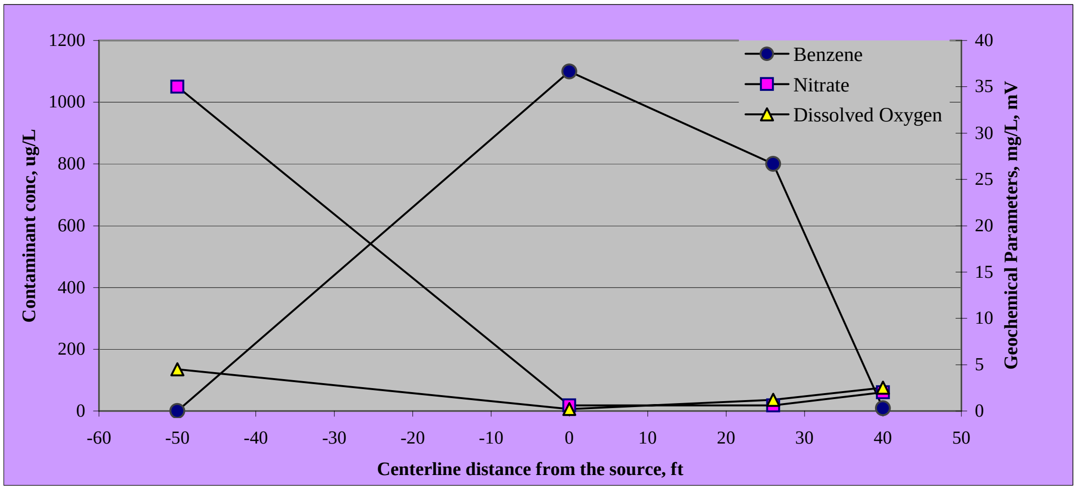
Contaminant for UF Selection **Benzene**

Equivalent Contaminant Degradation

		Unit	**UF**	NA	NA	MW-5	Mw-1	Mw-7	Mw-6	NA	NA	NA	NA	NA	NA
Dissolved Oxygen	utilized	mg/L	0.33	N/A	N/A	0.0	1.4	1.1	0.7	N/A	N/A	N/A	N/A	N/A	N/A
Nitrate	utilized	mg/L	0.21	N/A	N/A	0.0	7.2	7.2	6.9	N/A	N/A	N/A	N/A	N/A	N/A
Sulfate	utilized	mg/L	0.22	N/A	N/A	0.0	12.6	4.4	-0.4	N/A	N/A	N/A	N/A	N/A	N/A
Manganese	produced	mg/L	0.09	N/A	N/A	0.0	2.0	0.7	0.3	N/A	N/A	N/A	N/A	N/A	N/A
Ferrous Iron	produced	mg/L	0.047	N/A	N/A	0.0	4.1	2.0	1.1	N/A	N/A	N/A	N/A	N/A	N/A
Methane	produced	mg/L	1.3	N/A	N/A	0.0	10.4	6.6	5.5	N/A	N/A	N/A	N/A	N/A	N/A
Total		mg/L		0.0	0.0	0.0	37.7	22.1	14.0	0.0	0.0	0.0	0.0	0.0	0.0

4. Geochemical Indicator Plot

Hazardous Substance: Benzene
Geochemical Indicator? Dissolved Oxygen
Geochemical Indicator? Nitrate



Appendix F

Symbols and Abbreviations

Definition, abbreviation, and dimension of all symbols used in equations and tables of this document can be found in this Appendix F unless stated otherwise.

Note: Unit of symbols is described as a dimension: T (time), M (mass), L (length);
"Module" means a module contained in the Data Analysis Tool Package.

Abbreviations:

BTEX: Benzene, Toluene, Ethylbenzene, and Xylenes
C.L.: Confidence Level
CL_{calc}: Confidence Level; calculated for a specific data set
$CL_{DecisionCriteria}$: Predetermined Confidence Level; used as a decision criterion
CV: Coefficient of Variation; to account for the magnitude of scatter in the data
MTBE: Methyl Tertiary-Butyl Ether
NA: Not Applicable
NAPL: Non Aqueous Phase Liquid
TBA: Tertiary-Butyl Alcohol
TMB: Trimethylbenzene

Basic Hydrology Terms:

K: Hydraulic conductivity; (L/T)
i: Hydraulic gradient; (L/L)
n_e: Effective porosity; (dimensionless)
ρ_b: Dry soil bulk density; (M/L^3)

Concentration Terms:

C_o: Initial dissolved contaminant concentration at source zone at "*t* = 0"; (M/L^3)
$C_{x,y,z,t}$: The concentration of the contaminant at location x, y, z from the source at time "*t*"; (M/L^3)
C_{start}: Starting ground water concentration measured at a specific time and a specific monitoring well location; (M/L^3)
C_{CUL}: Ground water cleanup level; (M/L^3)

Dimension Terms:

1-D: One Dimension
2-D: Two Dimension
3-D: Three Dimension

Dispersion Terms:

α_x: Longitudinal (x-direction) dispersivity; (L)
α_y: Transverse (y-direction) dispersivity; (L)
α_z: Vertical (z-direction) dispersivity; (L)
D_x: Coefficient of hydrodynamic dispersion (x-direction); (L^2/T)
D_y: Coefficient of hydrodynamic dispersion (y-direction); (L^2/T)
D_z: Coefficient of hydrodynamic dispersion (z-direction); (L^2/T)

Mathematical Functions:

erf : Error function

$erfc$: Complementary error function

$\exp$: Exponential function

Model Area terms:

W : Modeled area length; (L); Refer to Module 6 for a detailed discussion.

L : Modeled area width; (L); Refer to Module 6 for a detailed discussion.

L_p : Estimated plume length; (L)

Model Coordinate Terms:

x : Plume centerline distance from the source, x-direction; (L)

y : Off-centerline distance, y-direction; (L)

z : Vertical distance from the centerline, z-direction; (L)

Rate Constants:

k_{point} : Point decay rate (1st-order) constant; (1/T):

- calculated from the slope of plot log of concentrations vs. time for a single monitoring point, slope of best-fit line;
- under Module 2, rate and time to achieve the cleanup goal with both best-fit and pre-determined level of confidences will be calculated for each well;
- refer to Module 2 for a detailed discussion of this parameter.

k : Bulk attenuation rate (1st-order) constant; (1/T):

- calculated from natural log of concentrations vs. distance for a overall stable or shrinking plume;
- need the locations of multiple wells from the sources and site specific ground water seepage velocity and retardation factor;
- rate with both best-fit and pre-determined level of confidences will be used to estimate a plume trend (how far a plume will expand);
- refer to Modules 2 and 5 for a detailed discussion of this parameter.

λ : Biodegradation rate constant; (1/T):

- calculated from the calibration of a ground water solute transport modeling that includes dispersion and retardation by adjusting "λ";
- refer to Modules 5 and 6 for a detailed discussion of this parameter.

k_{source} : 1st-order decay term for source concentration; (1/T):

- refer to Module 6 for a detailed discussion of this parameter.

Regression Terms (dimensionless):

n : Number of data used for log-linear regression

r^2 : Coefficient of determination of log-linear regression

r : Correlation coefficient of log-linear regression

CL: Confidence Level: refer to Module 2 for a detailed discussion of this term
CV: Coefficient of Variation: refer to Module 1 for a detailed discussion of this term

Sorption Terms:
R: Retardation Factor; (dimensionless)

$$R = 1 + \frac{K_{oc} f_{oc} \rho_b}{n_e} \qquad \text{(Eq. F.1)}$$

K_{oc}: Soil organic carbon-water partitioning coefficient; (L^3/M)
f_{oc}: Soil fraction of organic carbon; (dimensionless)

Source Terms:
Y: Width of source area; (L)
Z: Depth of source area; (L)

Time Terms:
t: Travel or restoration time; (T)
Δt: Average travel time between two control planes; (T)
$t_{1/2}$: Half life of a contaminant (1st-order kinetics); (T)

$$t_{1/2} = {\ln(2)}/{\lambda} = {0.693}/{\lambda} \qquad \text{(Eq. F.2)}$$

Velocity Terms:
v_{gw}: Ground water seepage velocity or average linear velocity; (L/T)
v_c: Contaminant velocity in ground water plume; (L/T):

$$v_c = {v_{gw}}/{R} \qquad \text{(Eq. F.3)}$$