

US EPA ARCHIVE DOCUMENT

4.0 3MRA Installation and User's Guide

The 3MRA modeling system is designed to execute on Personal Computers running the Microsoft Windows 95/98/2000/NT operating systems. This section describes the installation (Section 4.1), execution (Section 4.2), and simulation output review (Section 4.3) of the 3MRA modeling system.

4.1 Installing the 3MRA Modeling System

Installation of the modeling system for the Windows-based operating systems is managed by a single installation program located on the 3MRA installation disk. The following two sections present the specific sequence of installation steps for the 3MRA modeling system and a description of the directory structure (on the PC harddrive) containing the modeling software.

4.1.1 Installation Steps

To initiate the installation the user inserts the installation CD and, from the START/RUN menu locates and invokes the file setup.exe on the installation disk (e.g., E:\setup.exe). Figures 4.1 and 4.2 illustrate the opening screens of the InstallShield Wizard. The installation program prepares the system for installation by copying installation files to the users temporary file space (e.g., C:\Temp). Once prepared for installation, a Welcome screen appears (Figure 4.2). At all times during the installation the user is provided options to return to a previous screen, continue to the next screen, or cancel the installation.

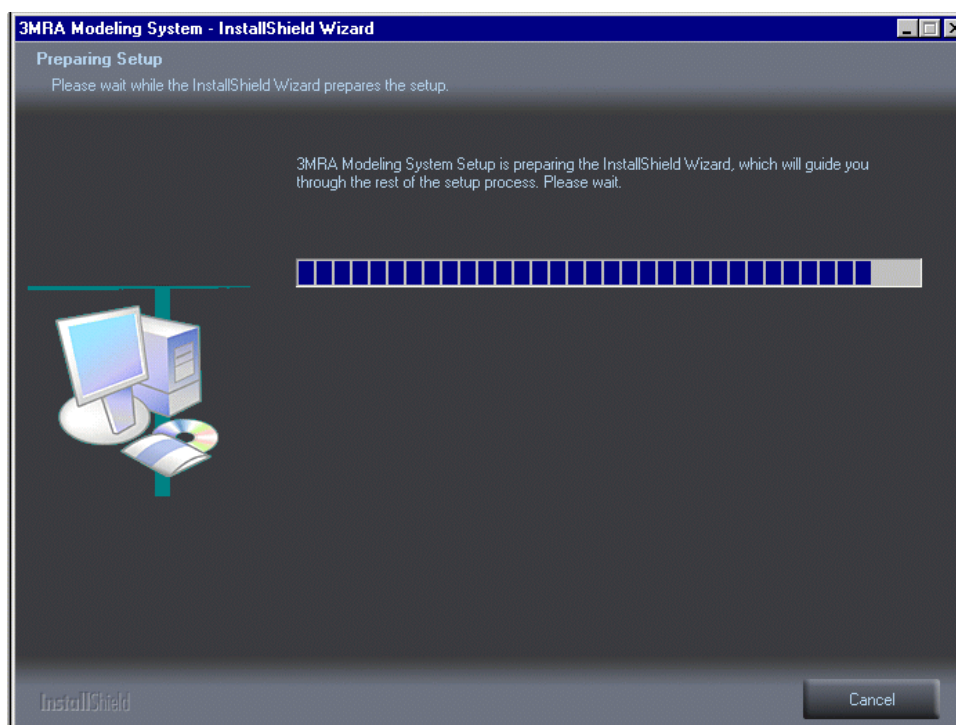


Figure 4.1 Opening Screen of 3MRA Installation Program

Figure 4.3 displays the licensing agreement that must be agreed upon by the user before installation of the modeling system will proceed. The 3MRA modeling system software is “open source”, that is, all materials related to the modeling system (i.e., program code, executables, databases, testing packages, and documentation) are available without charge to the public.

Figure 4.4 displays information concerning two options for installation; “Typical” and “Custom”. The Typical installation installs three items; 1) the 3MRA modeling system files, i.e., all executable programs and databases, 2) a set of database connectivity tools for 3MRA components that have been compiled using the Borland Compiler, and 3) a Java Runtime

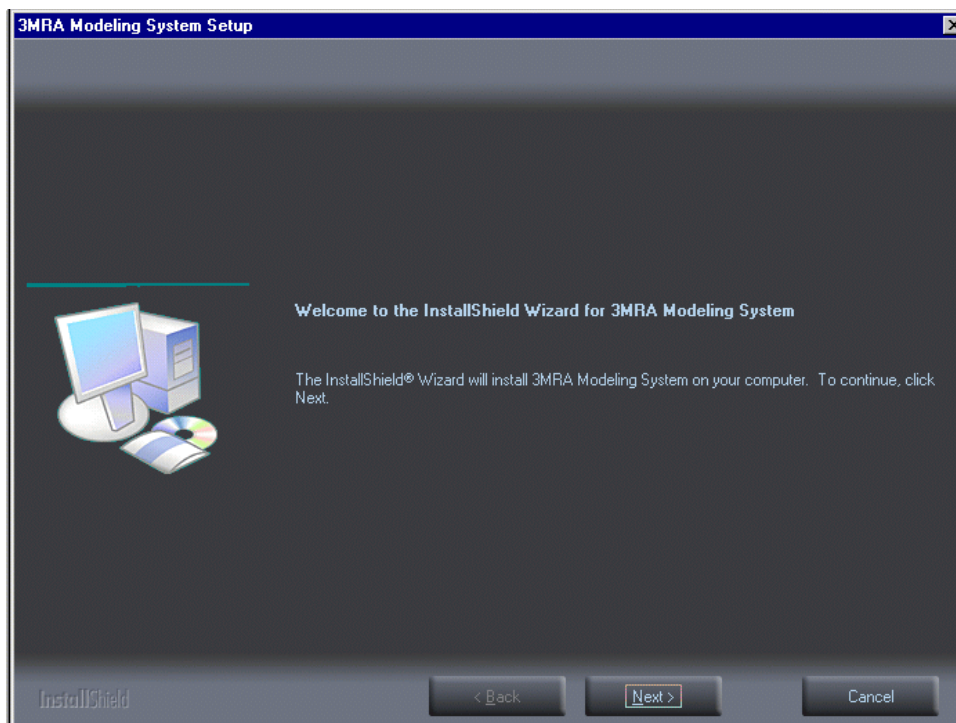


Figure 4.2 3MRA Installation Welcome Screen

Environment needed to run the Site Visualization Tool (SVT) that is written in Java. A Custom installation provides additional database connectivity files that may be needed for older versions of Windows (e.g., WIN95). Specific information concerning the need for Custom files is displayed in Figure 4.4. Figures 4.5 and 4.6 display the user installation selection options and associated information for Typical and Custom installation, respectively. Figure 4.7 displays the user screen for selecting/deselecting the various custom items.

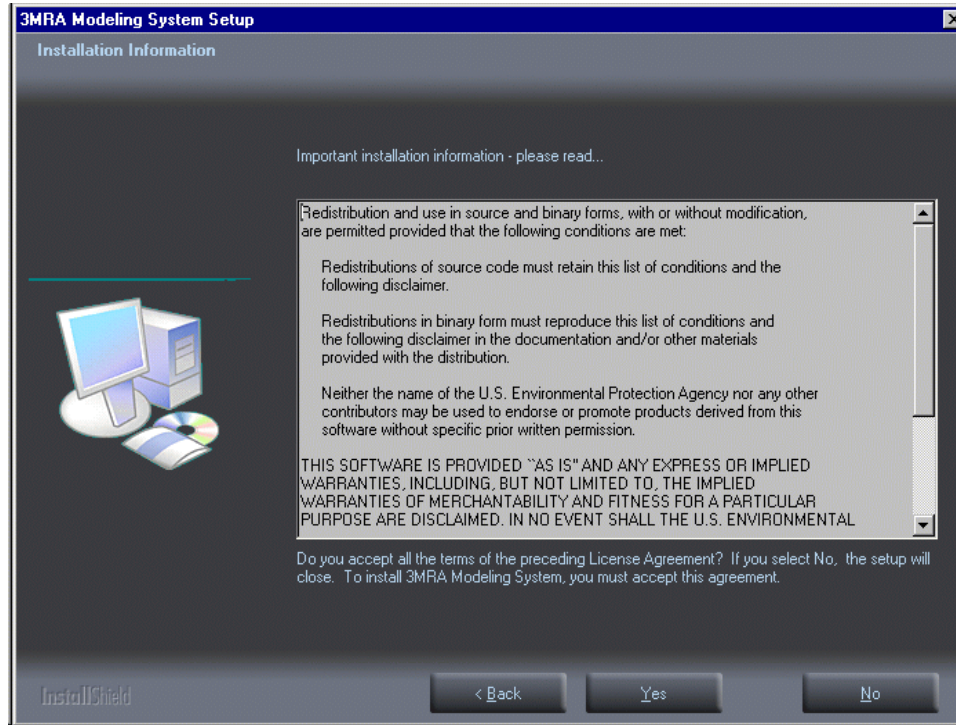


Figure 4.3 3MRA Licensing Agreement

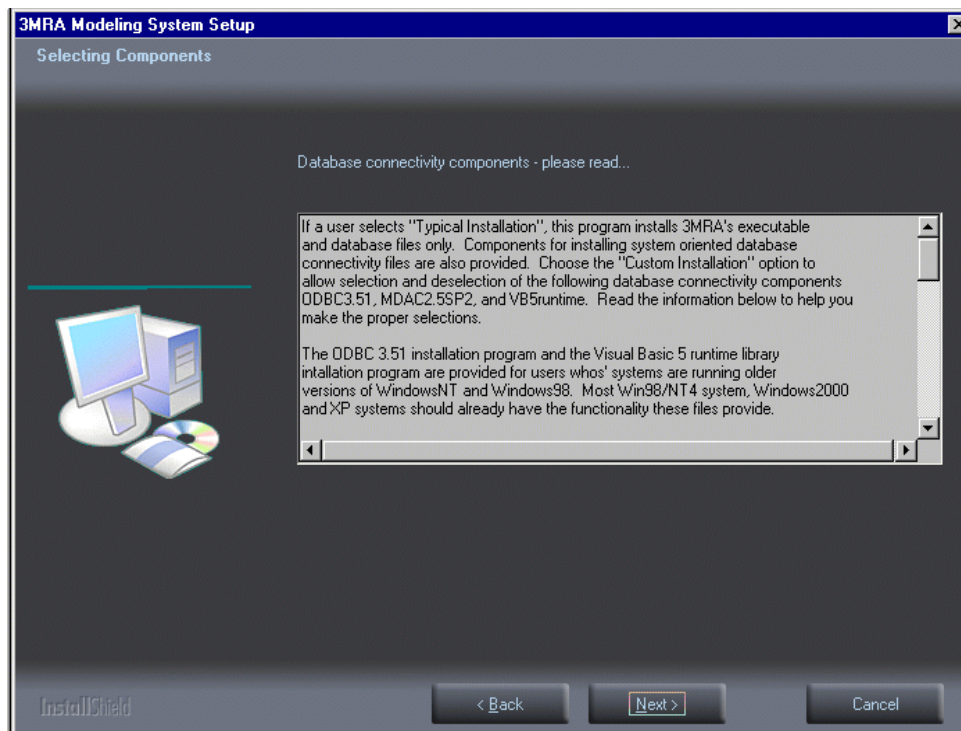


Figure 4.4 Description of 3MRA Installation Options

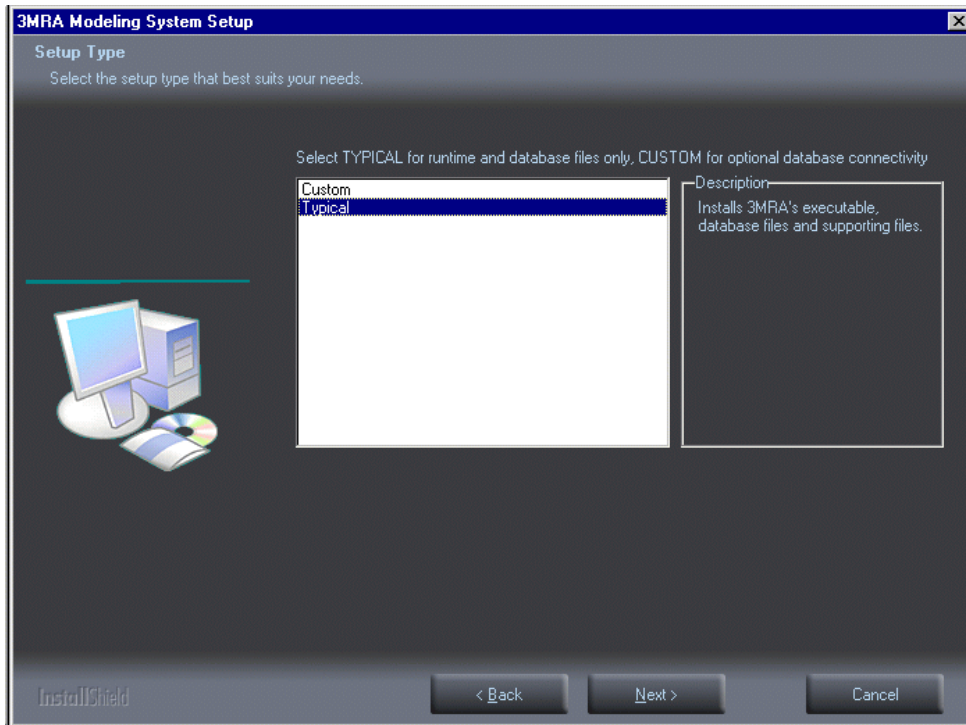


Figure 4.5 3MRA Installation Selection Screen : Typical

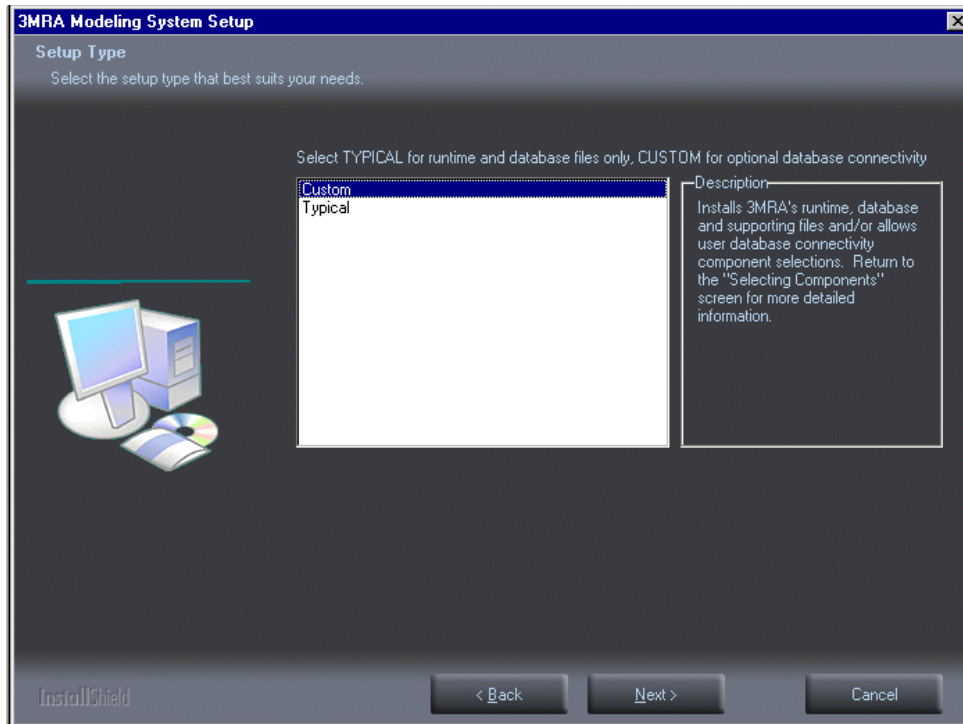


Figure 4.6 3MRA Installation Selection Screen : Custom

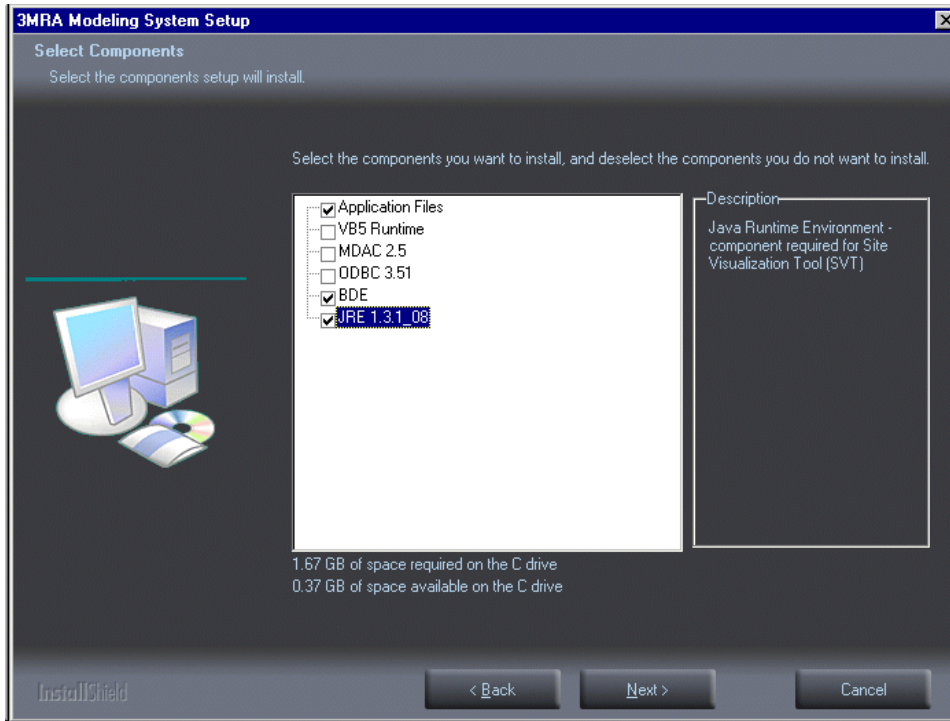


Figure 4.7 3MRA Installation Options for Database Connectivity Tools

Figure 4.8 displays the user screen for selecting the directory within which the 3MRA modeling system will be installed. Figure 4.9 displays a screen that communicates progress toward installing the modeling system.

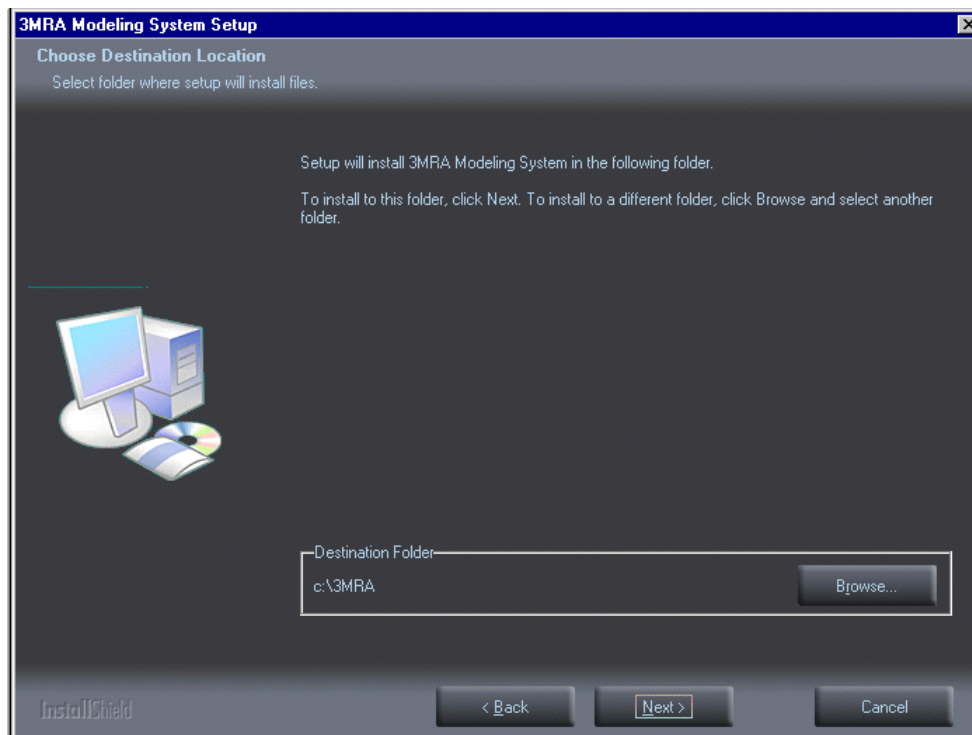


Figure 4.8 3MRA Installation Target Directory

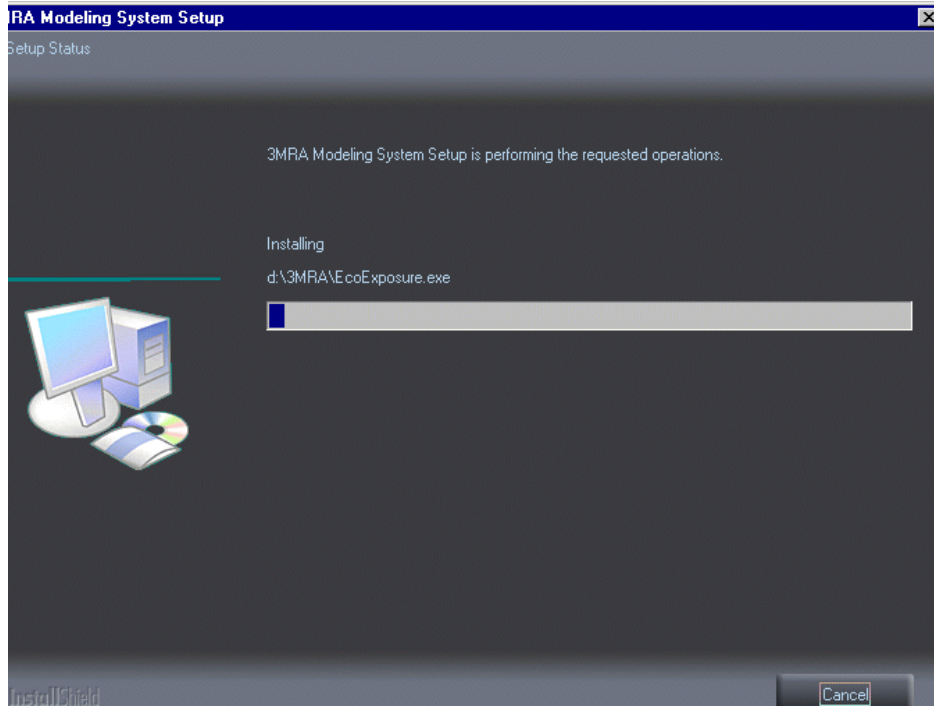


Figure 4.9 3MRA “Installation in Progress” Screen

Figures 4.10 through 4.13 display screens associated with installing the Java Runtime Environment (JRE). Figure 4.10 informs the user that the JRE installation files are being extracted and readied for installation. Figure 4.11 displays the Licensing agreement for the JRE. Figure 4.12 displays the installation screen for selecting the directory location for installation. It is recommended that the default directory, shown on the screen, be selected for installation. Figure 4.13 displays the screen for selecting the Browser to be used to display SVT graphical outputs.

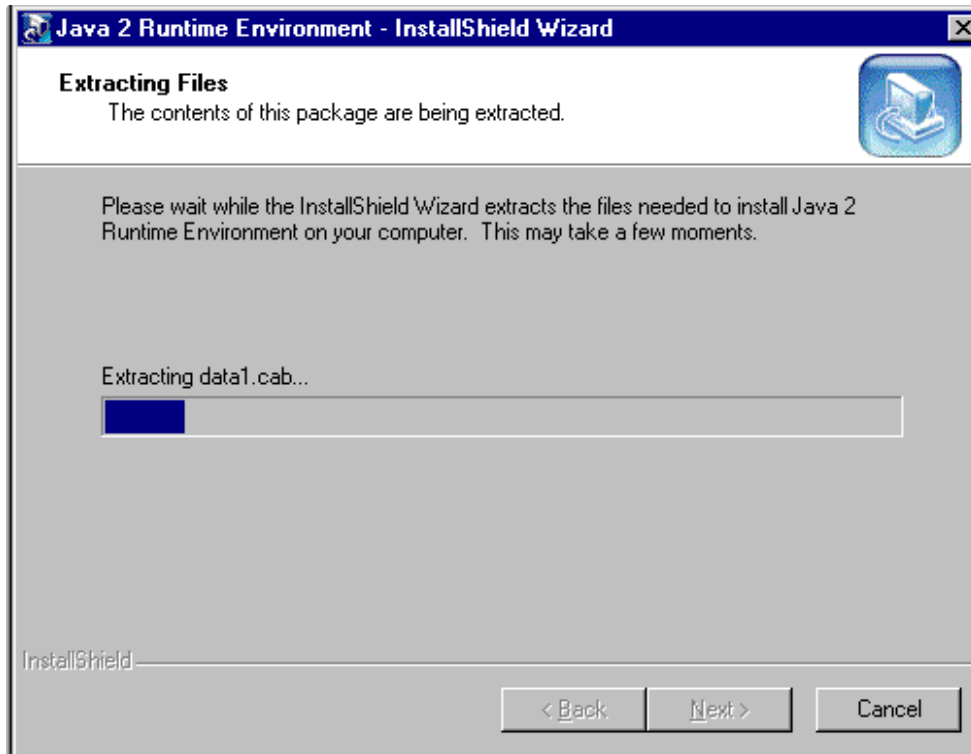


Figure 4.10 Java Runtime Environment Setup Screen

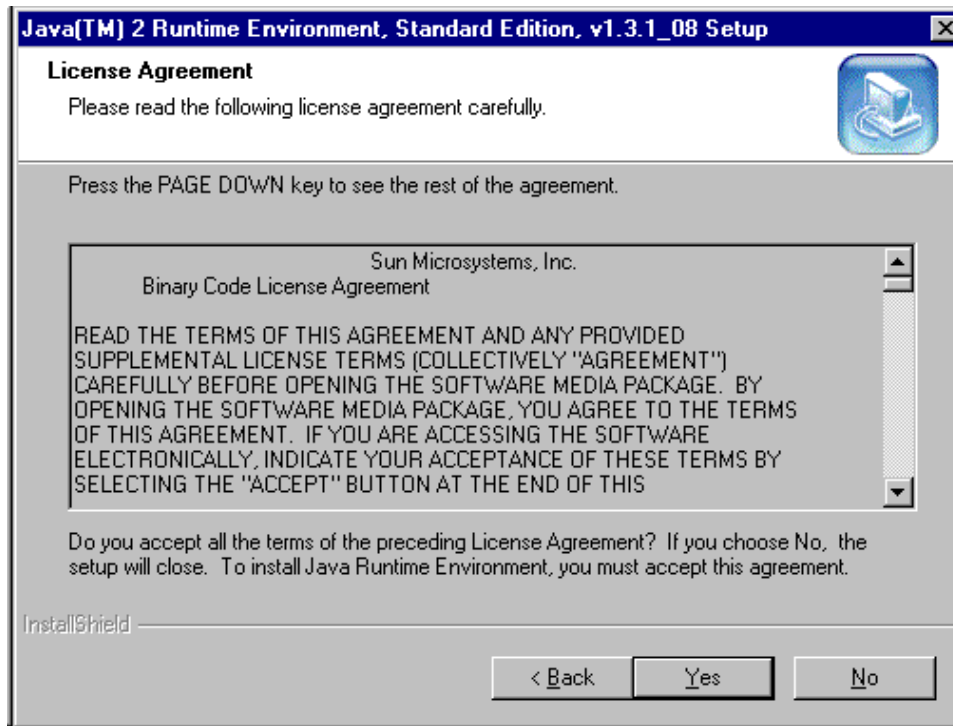


Figure 4.11 Java Runtime Environment Installation Screen

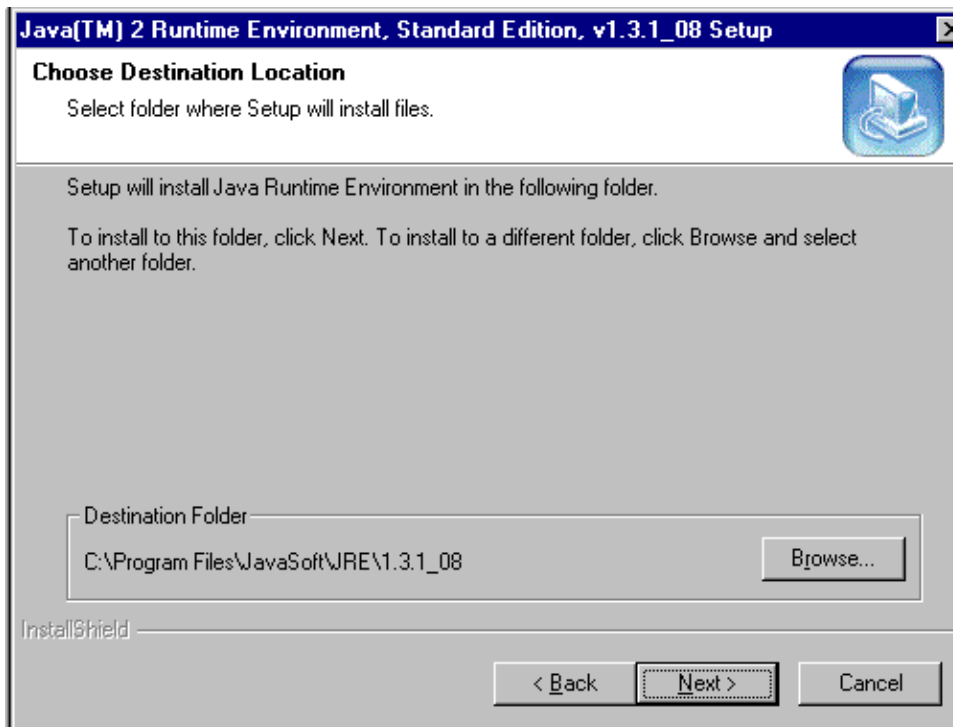


Figure 4.12 Java Installation Target Directory Screen

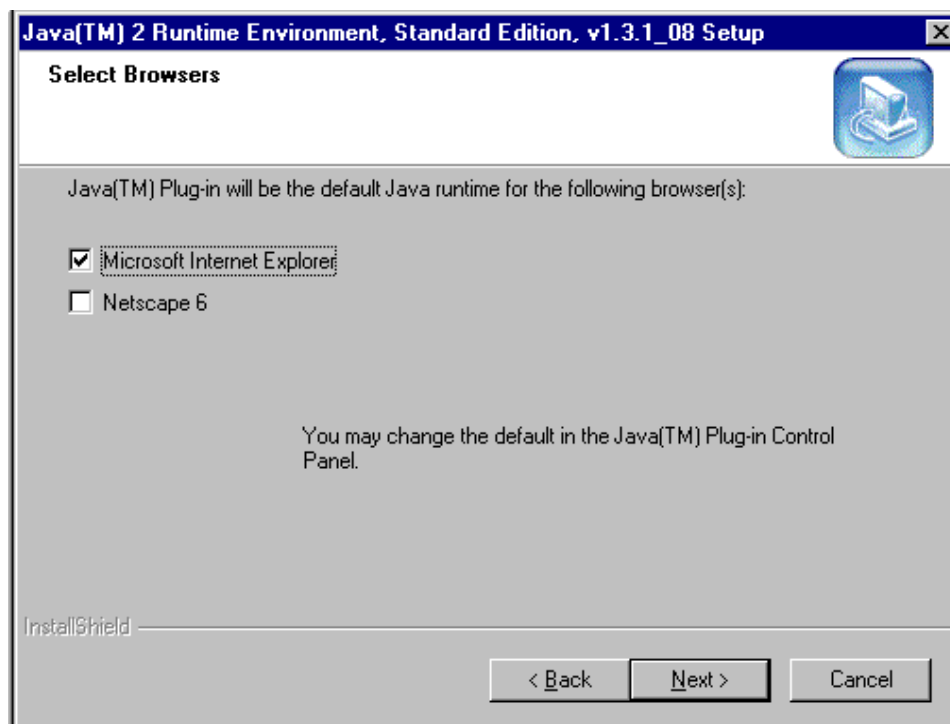


Figure 4.13 Java Runtime Browser Selection Screen

Figure 4.14 displays the final installation screen that informs the user that files containing directory path information have been modified to conform to the users directory specifications.

At this point the installation is complete and the user can proceed to invoke the 3MRA modeling system by clicking the START menu and PROGRAMS/3MRA/SUI.

Subsequent invocations of the 3MRA installation software begin with the screen shown in Figure 4.15. This screen allows user the following selections : 1) Adding or removing components (as in a "Custom" setup) with "Modify", 2) Reinstalling the components previously installed with "Repair", or 3) Removing the installation with "Remove". If the user selects "Remove" only those 3MRA files originally installed will be removed. Files that have been generated by the user, e.g., from performing simulations, will remain, along with the associated directory structure.

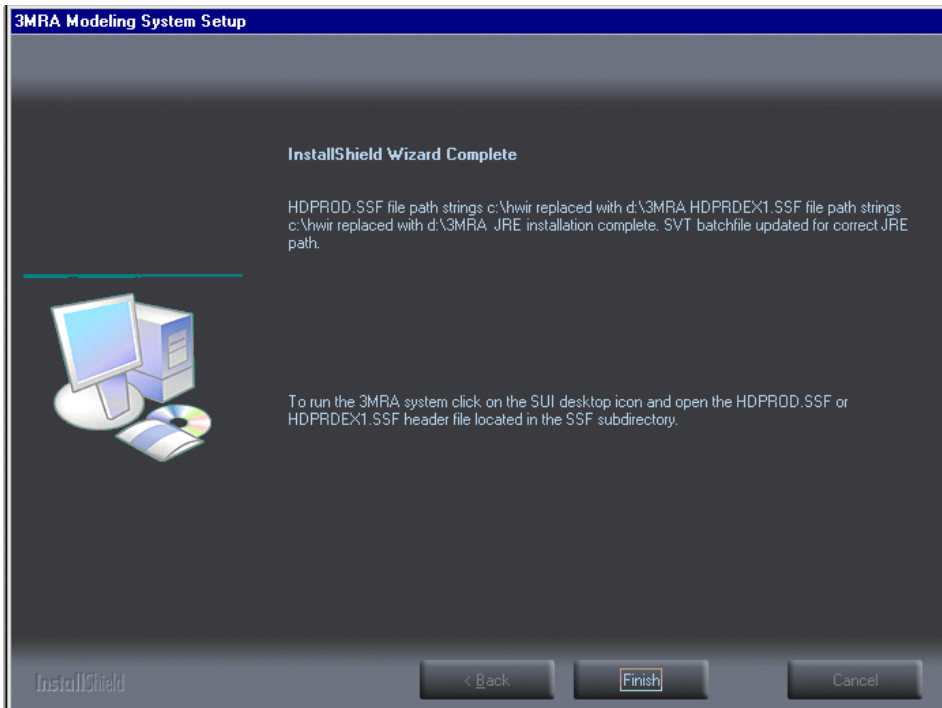


Figure 4.14 3MRA Final Installation Screen

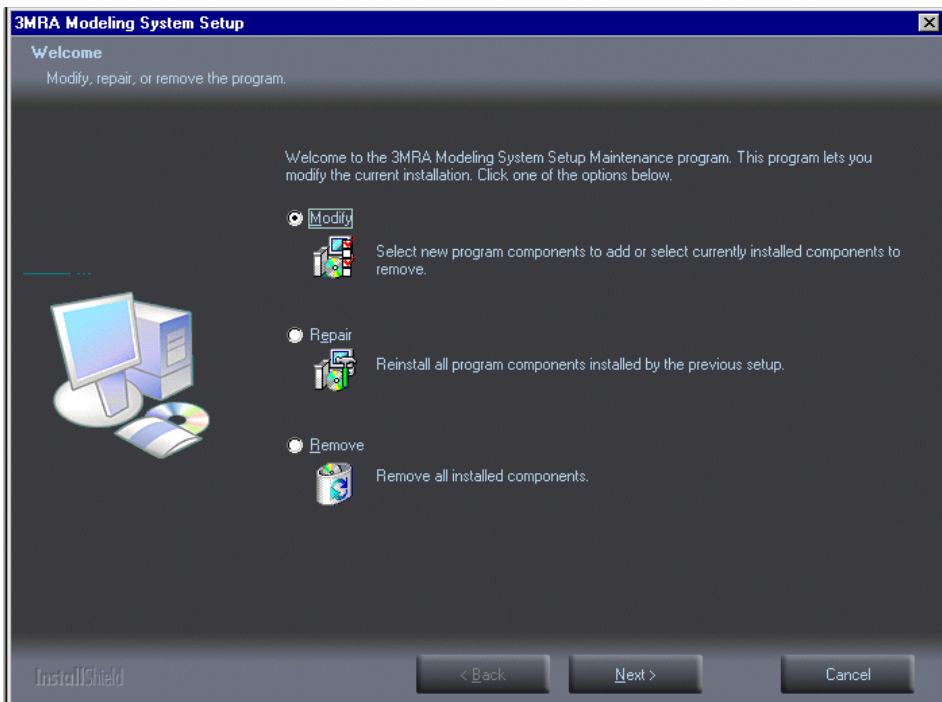


Figure 4.15 3MRA Modify/Repair/Remove Installation Screen

4.1.2 Directory Structure for 3MRA

Upon completion of the 3MRA modeling system installation the complete set of files needed to execute the system are placed onto the user specified harddrive (e.g., C:\). Figure 4.16 illustrates the Directory structure assuming the 3MRA modeling system has been installed on D:\3MRA. The root directory (i.e., D:\3MRA) contains all the executable components of the modeling system, including the seventeen science modules and the system processors. Below the 3MRA directory are a series of subdirectories containing 3MRA databases, example simulation output files, and software for the Site Visualization Tool (SVT) that facilitates visualization of single site output GRF files. The following discussion provides a description of the contents of each of the 3MRA subdirectories.

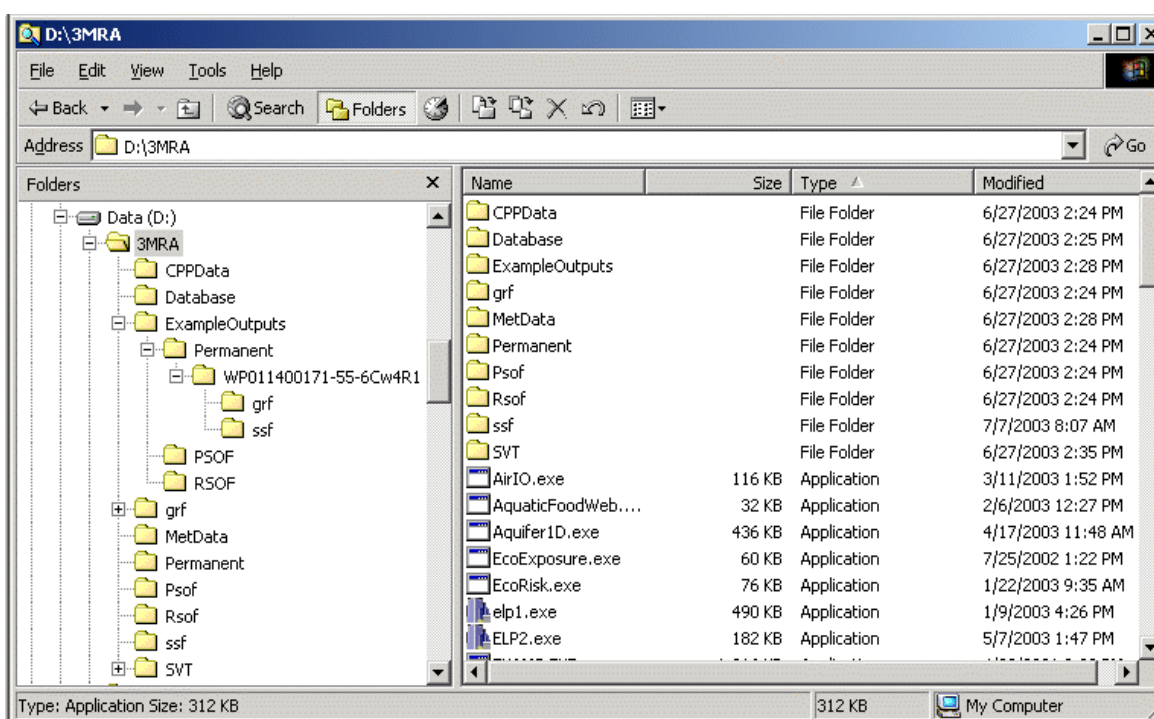


Figure 4.16 3MRA Directory Structure after Installation

Figure 4.17 illustrates the contents of the Chemical Properties Data subdirectory (D:\3MRA\CPPData). There are 15 individual chemical property files, each containing a specific type of chemical data. The data files are comma separated ASCII data files and can easily be viewed using a spreadsheet program (e.g., Microsoft Excel).

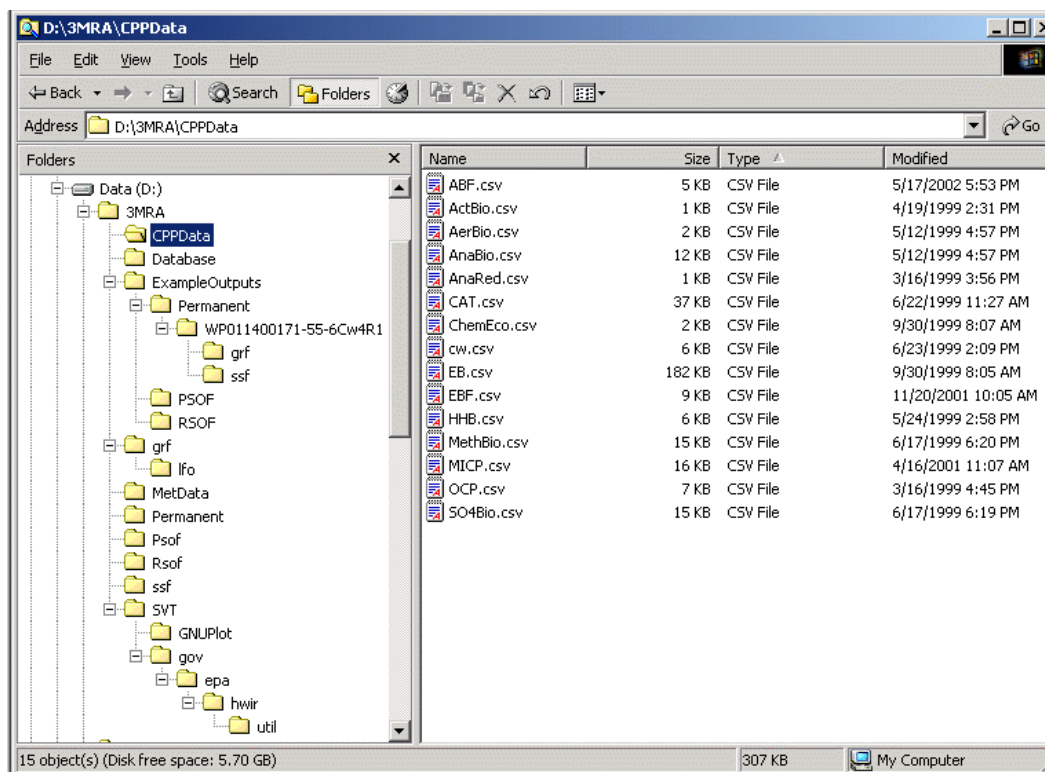


Figure 4.17 3MRA Directory Structure : CPPData Subdirectory

Figure 4.18 illustrates the contents of the D:\3MRA\Database that contains the three main data files needed to populate the Site Simulation Files (SSFs). The three data files (Site, Regional, and National) are Microsoft Access data files and can be viewed and edited with this program.

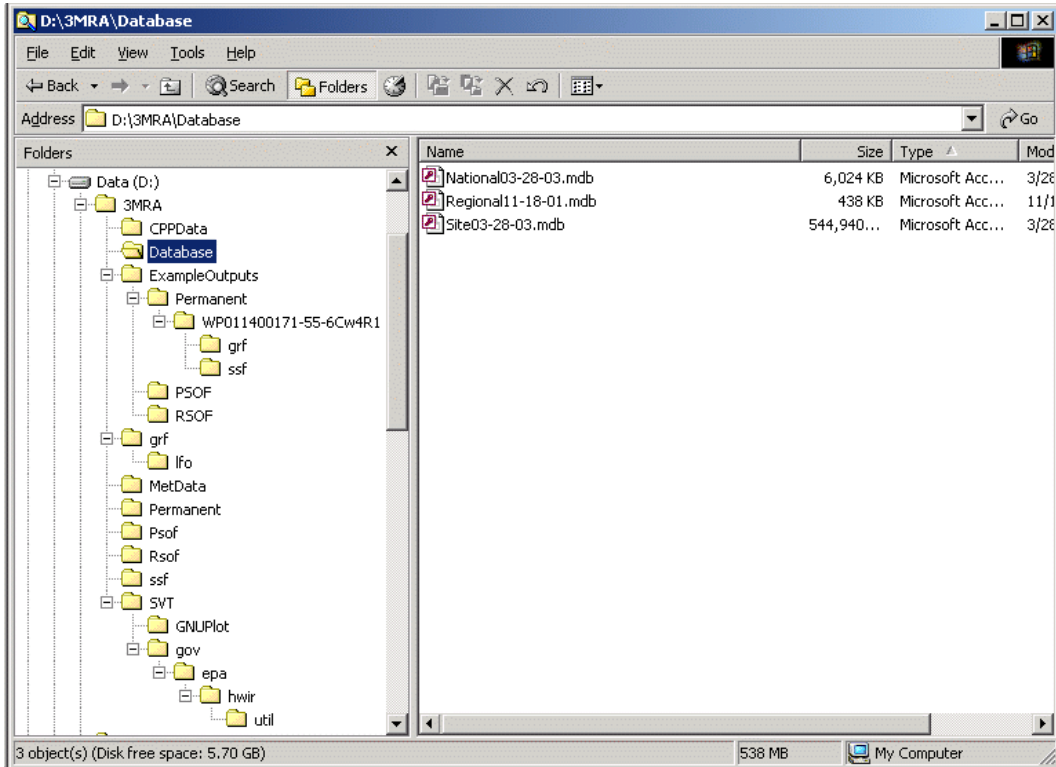


Figure 4.18 3MRA Directory Structure : Database Subdirectory

Figure 4.19 illustrates the contents of the D:\3MRA\ExampleOutputs directory. This directory contains the results of two 3MRA simulations; a set of results for a single site simulation and results from a national simulation to establish exemption levels for benzene. The Permanent subdirectory contains the results for a 3MRA simulation where a single site/chemical/WMU/Cw was selected. When the results for individual sites are saved the 3MRA modeling system places the resulting GRF and SSF files in subdirectories under a directory named for the site simulation (for example, as shown in the figure the subdirectory “WP011400171-55-5Cw4R1”, this simulation involved a Waste Pile (WP), at site number 0114001, for the chemical whose CAS number is 71-55-6, and for Cw number 4. These example site simulation results are included in the 3MRA modeling system installation to allow the user to execute the Site Visualization Tool (SVT) described in Section 4.3.

Additionally, the ExampleOutputs directory contains subdirectories “PSOF” and “RSOF”. The RSOF subdirectory contains the results of a national simulation that includes all sites, all WMUs, and all Cw’s for the chemical benzene. Thus, the data files contained in the RSOF subdirectory can be used to execute the ELP II processor (See Section 4.3). Results of running the ELP II are tables listing national exemption levels. These results are stored in the PSOF subdirectory.

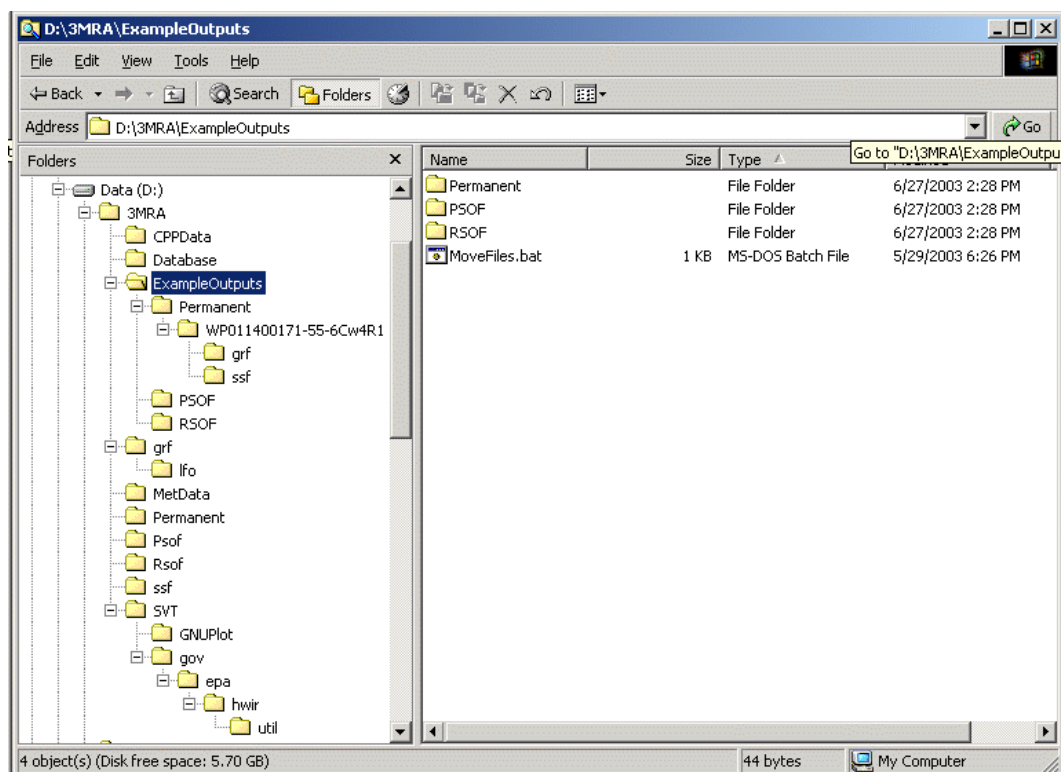


Figure 4.19 3MRA Directory Structure : ExampleOutputs Subdirectory

Figure 4.20 illustrates the contents of the D:\3MRA\grf subdirectory. Included in this subdirectory are the DICTIONARY files for each of the GRFiles associated with the 3MRA science modules. These files are ASCII data files and can be viewed with any TextEditor (e.g., WordPad – do not edit these files with a Word Processor). Also contained in the GRF subdirectory is the “lfo” subdirectory that contains the normalized output files of the atmospheric module for each site and WMU combination. These files are created the first time the atmospheric module is executed for a site/WMU combination. Any subsequent simulations that include this site/WMU combination will by-pass the atmospheric module and process the normalized data contained in these data files.

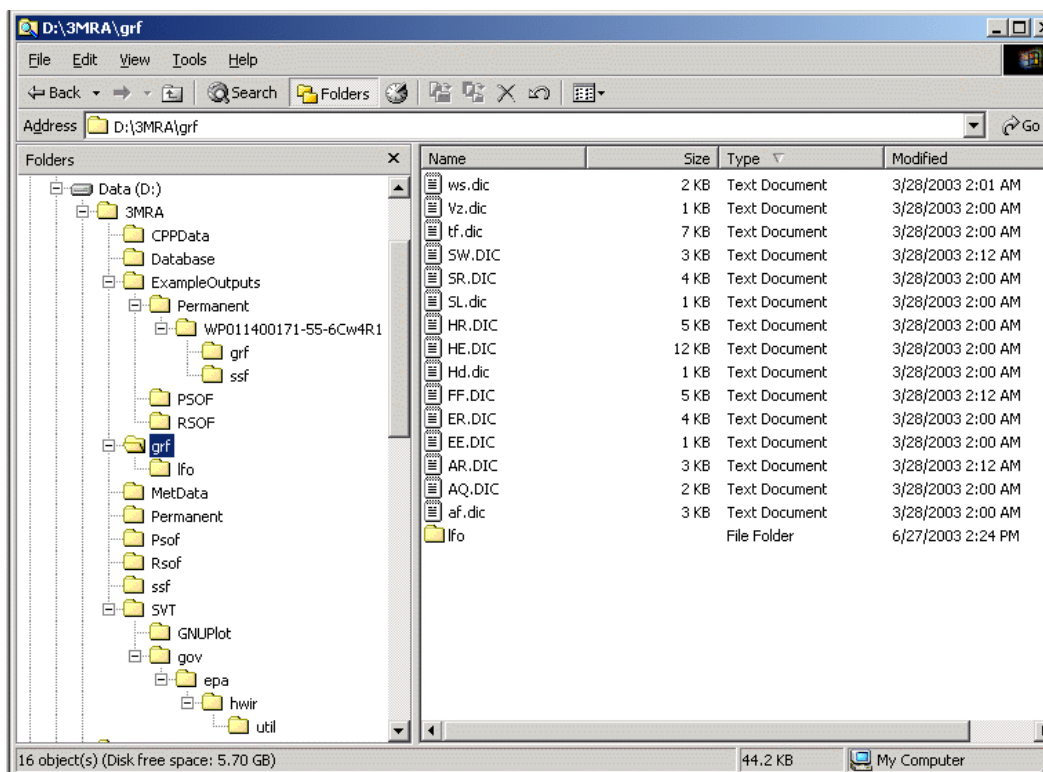


Figure 4.20 3MRA Directory Structure : GRF subdirectory

Figure 4.21 illustrates the contents of the D:\3MRA\MetData subdirectory. All meteorological data files are contained here, including hourly, daily, monthly, annual, and long-term average data. These data files are ASCII data files and can be viewed with a TextEditor.

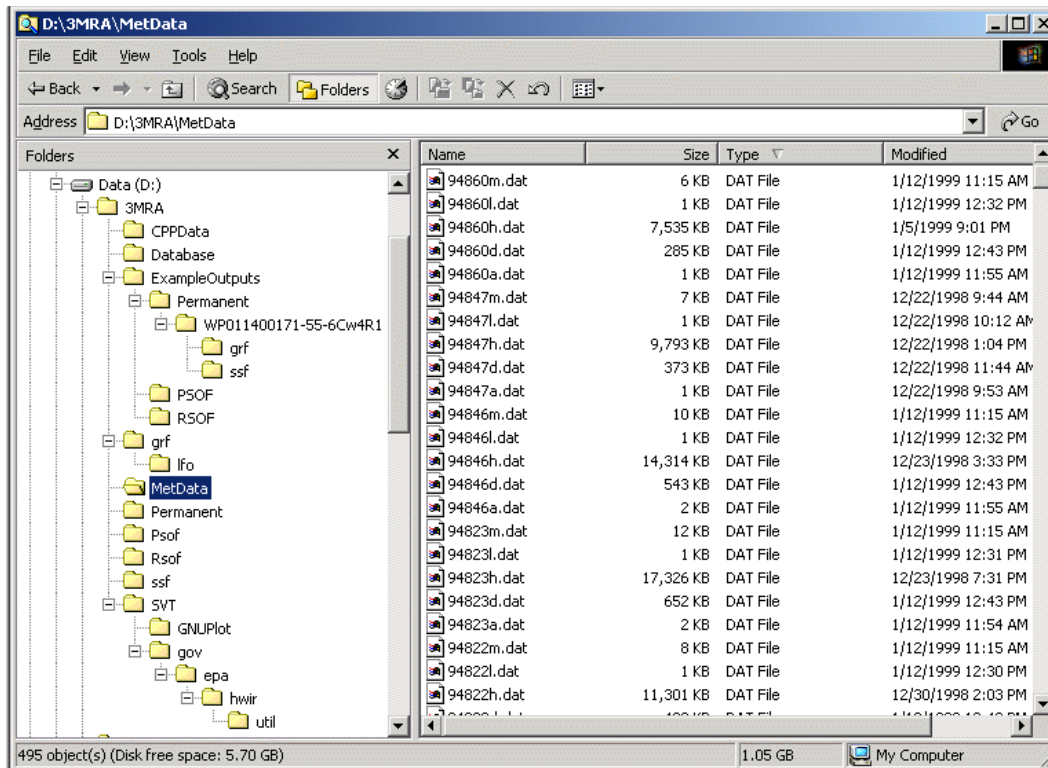


Figure 4.21 3MRA Directory Structure : MetData Subdirectory

Figure 4.22 illustrates the contents of the D:\3MRA\PSOF subdirectory. This subdirectory contains Microsoft Access database files that contain the standard (or user specified) regulatory “scenarios” (ELP2.mdb) and a database file that contains the table format for output results of executing the ELP II Processor. Also, contained in this subdirectory (but not shown here) are the actual tables produced by the ELP II. These files are produced in Microsoft Excel format.

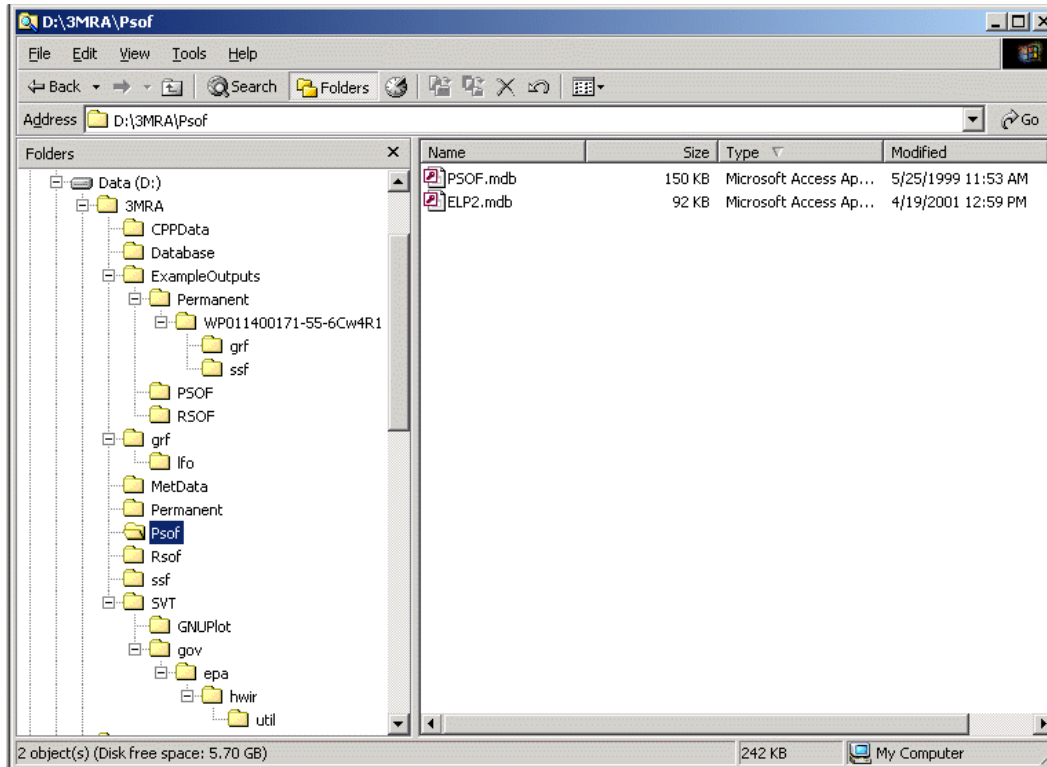


Figure 4.22 3MRA Directory Structure : PSOF subdirectory

Figure 4.23 illustrates the contents of the D:\3MRA\Rsof subdirectory. This subdirectory contains a Microsoft Access database file the includes “templates” that describe the Risk Summary Output File format. Not shown here (but included in the D:\3MRA\ExampleOutputs\Rsof subdirectory) are Microsoft Access database files containing the ELP I results from national simulations. These database files contain the input data for executing the ELP II Processor.

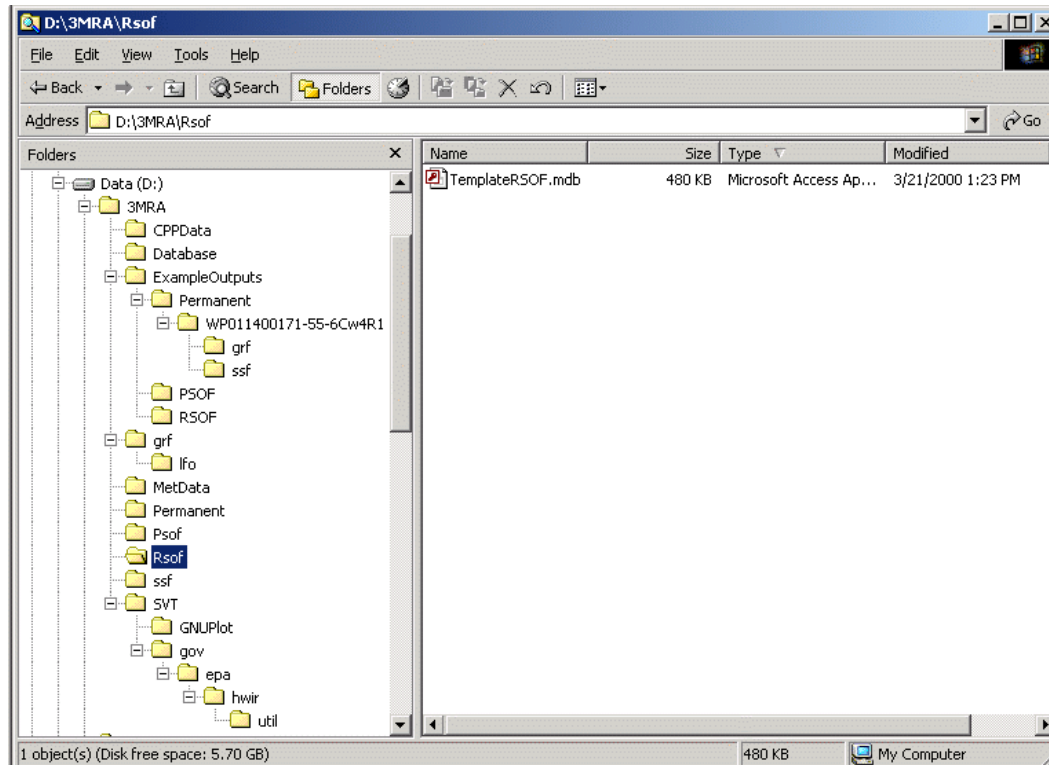


Figure 4.23 3MRA Directory Structure : Rsof subdirectory

Figure 4.24 illustrates the contents of the D:\3MRA\ssf subdirectory. This subdirectory contains the DICTIONARY files for the Site Simulation Files (SSFs). These files are ASCII data files and can be viewed with a TestEditor. This directory also contains the individual SSFs resulting from a 3MRA simulation.

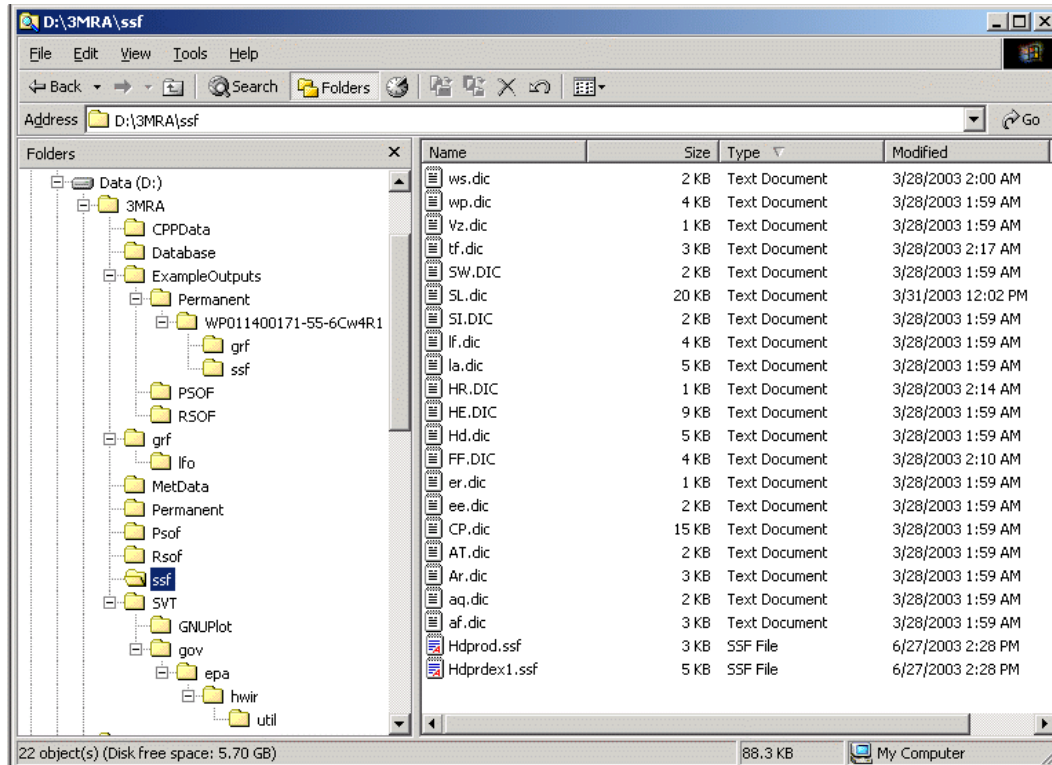


Figure 4.24 3MRA Directory Structure : SSF subdirectory

Figure 4.25 illustrates the content of the D:\3MRA\SVT subdirectory. This subdirectory contains the software related to the Site Visualization Tool. This software is used to produce time series plots for single site simulation results. This execution of this software is described in Section 4.3.

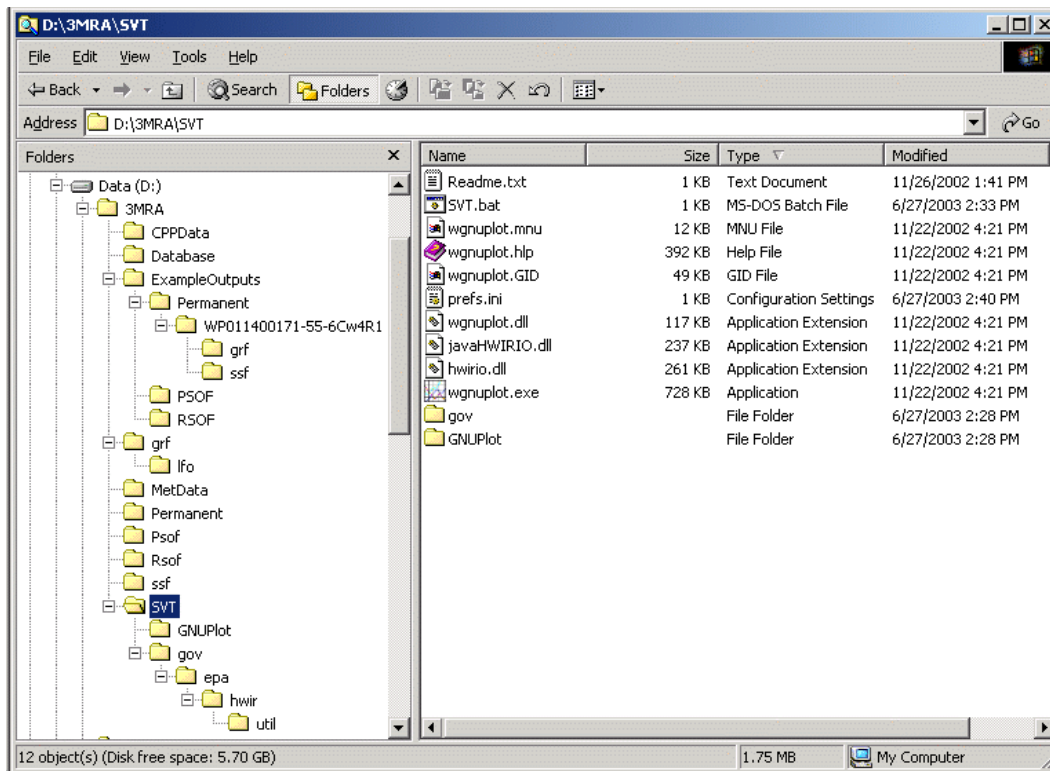


Figure 4.25 3MRA Directory Structure : SVT subdirectory

4.2 Executing the 3MRA Modeling System

This section describes the sequence of steps necessary to execute a 3MRA assessment.

A 3MRA assessment consists of a combination of chemical(s), site(s), waste management unit(s), wastestream concentration(s), and Monte Carlo iteration(s). The number of sites available for an assessment is dependent upon the WMUs selected. Each site contains one or more of the WMUs but no site contains all WMUs, thus, depending on the WMU selected the number of sites available will vary. The adjoining table lists the WMUs and the number of sites that contain the particular unit type. National scale assessments always include at least one WMU, all sites containing the WMU, all wastestream concentrations (Cw's), at least one chemical, and at least one Monte Carlo iteration. Typical national assessments include all combinations of sites and WMUs along with all Cw's and one chemical and one Monte Carlo iteration. The total number of site simulations in this case is 2095 (i.e., 419 site/WMU combinations times 5 Cw's). The typical national scale assessment takes on the order of 2 to 5 days for a modern Personal Computer (PC) to complete, depending on the chemical (less volatile, more hydrophobic chemicals remain in the environment near the source for longer periods of time, thus requiring more simulation time). The total number of simulations would scale proportionately for each additional chemical and Monte Carlo iteration (e.g., 100 Monte Carlo iterations would require a total of 209,500 individual site simulations). Note that each Monte Carlo iteration implies that the total set of site simulations will be repeated the specified number of times.

Waste Management Unit (WMU) Type	Number of Sites Containing WMU
Landfill	56
Land Application Unit	28
Surface Impoundment	137
Aerated Tank	137
Waste Pile	61
All WMU Types	419*

* There is a total of 419 combinations of WMU and site location.

Smaller scale assessments are typically conducted to either perform a test of the modeling system or, more typically, to review the results of a single site simulation. Any combination of 3MRA sites, chemicals, WMUs, Cws, and Monte Carlo iterations is possible. In the case when a user wishes to review the results of a single site the user may specify a single combination of a site, chemical, waste management unit, wastestream concentration, and a single Monte Carlo iteration. When executing a single site assessment it is possible to store the results of each science module. This provides the user with the ability to follow a simulation step by step from source release to risk.

NOTE: 3MRA Version 1.0 is not designed to facilitate the definition of “new” sites by the user. That is, there is no user interface that allows the user to input data associated with a new site. Sites currently contained in the Site Database represent a specific collection of sites used to conduct a national assessment of risks from land-based waste management disposal units. While it is possible to input a new site (i.e., non-3MRA national assessment site) the process requires intimate knowledge of the Microsoft Access database structure used for 3MRA. Information for defining new sites is not presented in this document. The next version of 3MRA will include a user interface to facilitate definition of new sites.

The combinations required for each assessment are communicated to the modeling system, by the user, via the System User Interface(SUI). The users view of the 3MRA modeling system is presented through a series of SUI menu screens that present simulation options to the user and accept user choices. Section 4.2.1 presents the complete set of SUI menu screens while sections 4.2.2 and 4.2.3 describe, by way of an example simulation, the output processing capabilities of the 3MRA modeling system. The first example is of a National assessment to establish an exemption level for benzene. The processing of National simulation results by the Exit Level Processor II/Risk Visualization Processor (ELP II/RVP) are described. The second example is the execution of a single combination of a site, chemical, waste management unit, and wastestream concentration level. The Site Visualization Tool (SVT), capable of producing time series plots of all science modules, is described.

4.2.1 System User Interface (SUI)

There are three main functions of the 3MRA System User Interface; system configuration, system management, and system status. The system configuration function defines the locations of all files required to run a simulation (database files and processor and module executables). This function also specifies where the data files that are produced by the system are to be stored. The system management function defines which sites, chemicals, source types, and waste levels are to be included in the simulation, as well as the storage level of output, the number of iterations, and the run mode. The system status function allows the user to start, stop, reset, and resume the simulation. It also reports any errors or warnings that may have occurred during the simulations.

The **SUI menu screens** include a few general features that facilitate information exchange between the user and the modeling system. These features, illustrated in Figure 4.26, include “tabs”, “buttons”, and “text windows”.

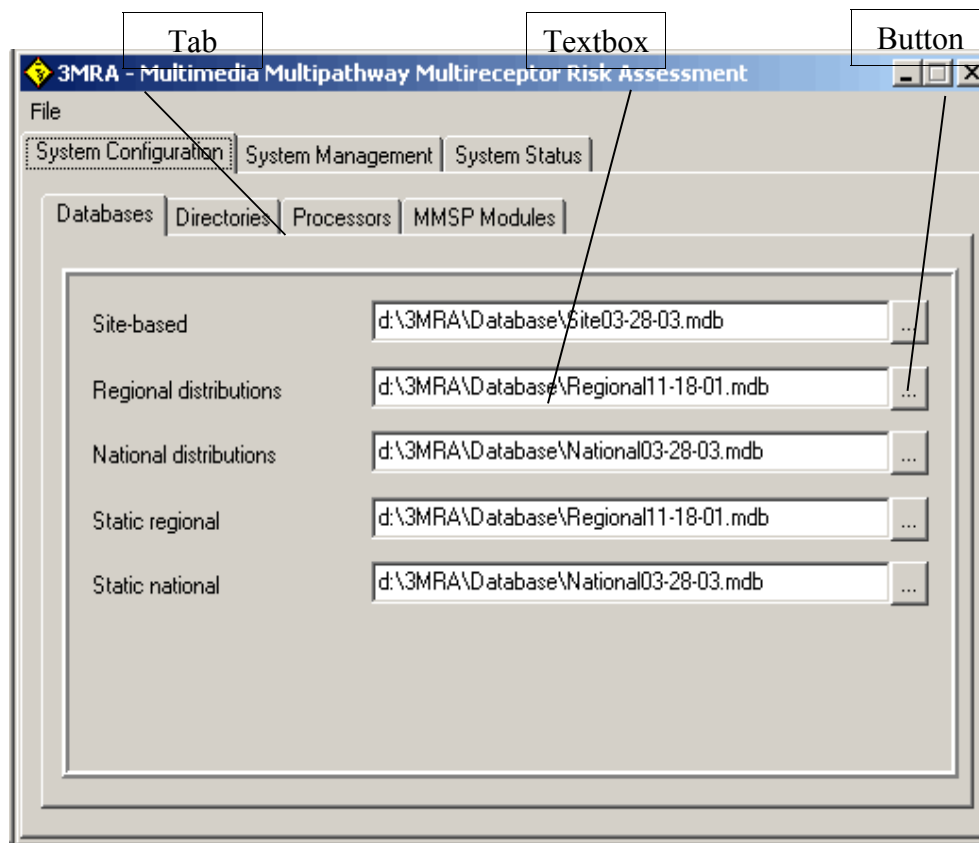


Figure 4.26 User Interaction Features of 3MRA Menu Screens

Tabs represent categories of data/information and when activated display a menu screen designed to present and gather information relevant to the data category. Tabs may simply represent options available to the user or they represent a logical hierarchical data structure. Tabs are activated with a single left click of the mouse.

Text windows accept information/data from the user in one of two ways. First, the user can simply type the relevant information/data directly into the window. The second type of text window is populated with information from the modeling system (e.g., a list of 3MRA sites) and requires the user to select specific entries.

Buttons invoke specific actions on the part of the SUI. There are only a few specific buttons included in the SUI. The button is used to browse file/directory locations. Upon a single click of this button the user is presented access to the directory of files on the host computer. This button is provided to facilitate the users population of specific text windows that require file name and directory location data. By double clicking on a file name it will appear (with all relevant directory relationships) in the text window. Other buttons include which invoke intuitive actions with respect to the simulation execution.

Pre Simulation Preparations

One final point before describing the SUI functionality. Subsequent to the initial simulation of the 3MRA modeling system but before each subsequent simulation it is recommended that the user run a clean up procedure to remove files left over from previous simulations. Double clicking on the 3MRACleanUp.bat file (shown in Figure 4.27) starts the cleanup routine. The routine deletes residual Site Simulation Files (SSFs) and Global Results Files (GRFs) as well as residual Risk Summary Output Files (RSOFs). In addition, it deletes Error and Warning files left from the previous runs. Lastly, the cleanup routine compares the files in the 3MRAVer1.txt manifest file to the files in the application folder. This check is to ensure that the official version of the 3MRA software system is installed. If, for example, the user has updated a database or modified a science module, the 3MRA system will no longer represent that which was installed. The cleanup procedure reports any differences by writing to the Messages.all file in the 3MRA:\GRF directory.

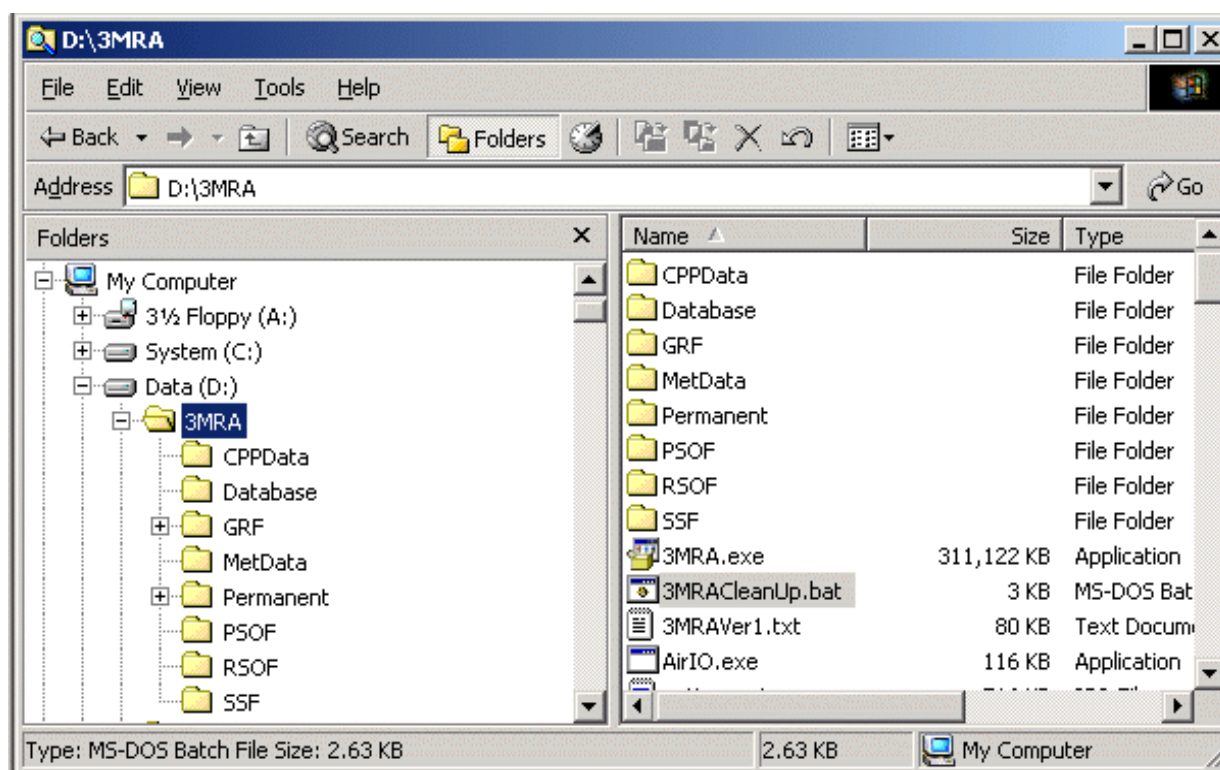


Figure 4.27 3MRA Directory Listing Displaying Batch File for System Cleanup

4.2.2 Invoking the 3MRA Modeling System

To invoke the 3MRA modeling system the user enters the Windows Start menu and selects PROGRAMS/3MRA/SUI. The first screen that appears is shown in Figure 4.28. The user then clicks on **File** and then **Open**. This opens the directory listing window for the purpose of having the user locate and identify the “header file” to be used to establish the default settings for the SUI (Figure 4.29). The header file contains all the information necessary for the modeling system to locate files, databases, science modules, and input/output files necessary to execute the 3MRA. Any information/data contained in the header file can be modified through the SUI. Under the standard installation procedure described in Section 4.1 the header file is located in C:\3MRA\SSF. The user locates this file, highlights the file by left clicking on it, and then clicking on the **Open** button (or simply double left clicks on this filename). The SUI then

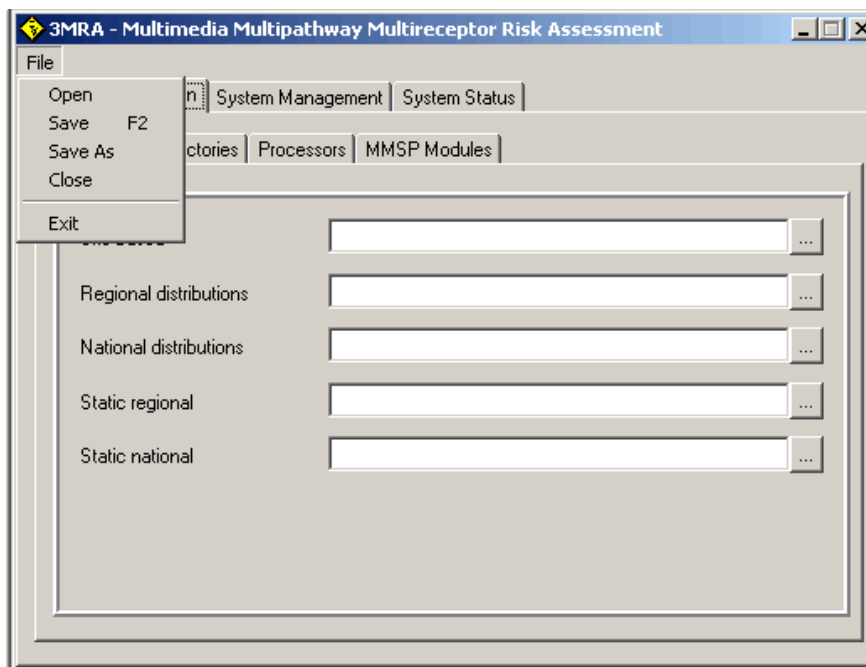


Figure 4.28 Initial 3MRA User Interface Screen

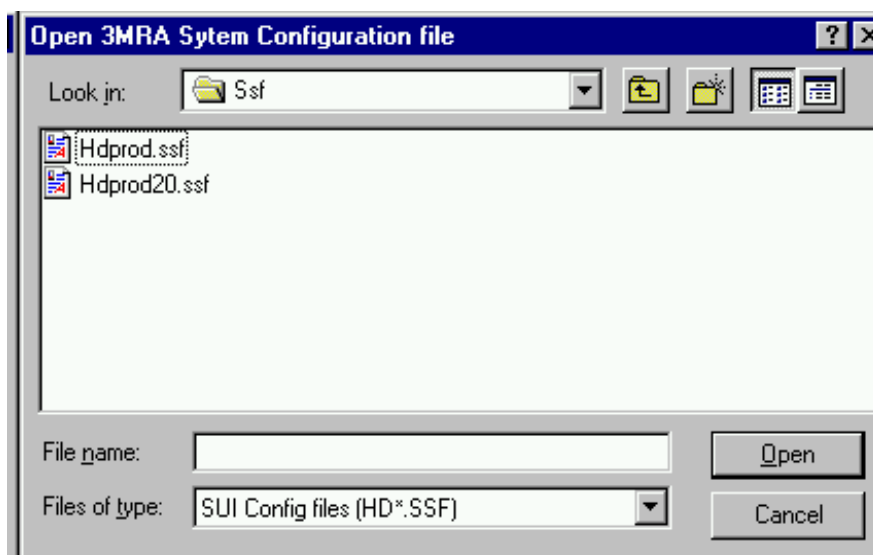


Figure 4.29 3MRA Header File Selection Screen


reads the file and populates all menu screens with appropriate data from the header file. From this point on the 3MRA menu screens will contain default information/data. If the user modifies any information, the updated header file can be saved by pressing the **File** key, and then the **Save as** key. It is convenient to save all header files in the same C:\3MRA\SSF file directory.

4.2.2.1 System Configuration

The system configuration function is managed through the SYSTEM CONFIGURATION SCREEN of the SUI that, in turn, has several additional subscreens linked with it. The primary purpose of the series of configuration screens is to allow the user to select and define the directory location of all files necessary to execute the 3MRA modeling system. When the “header file”, described in the previous section, is accessed and read by the SUI there is a complete set of file locations read and placed as defaults on the system configuration screens. So, in essence, the user rarely exercises these screens except to make modifications (e.g., the user wishes to use a module or database located outside the standard installation directories).

There are four main categories of file directory information required, represented by the second tier of tabs (subscreens) below the **System Configuration tab** in Figure 4.30 and including Databases, Directories, Processors, and MMSP Modules. Each of these categories are explained below with a graphic of the screen to aid understanding.

Databases SubScreen

The Databases subscreen shown in Figure 4.30 lists the site related databases required for 3MRA. While five site databases are listed on the screen only three are currently implemented in the 3MRA modeling system. The Site-based, Regional Distribution, and National Distribution databases are implemented and must be specified. As noted above the  button can be used to facilitate locating and assigning database files in the appropriate textboxes. The Static Regional and Static National are not currently utilized by the modeling system (they represent place holders for a future version of the modeling system) but must contain entries nonetheless. For purposes of convenience the Regional Distribution database and the National Distribution database are repeated here to allow the system to function.

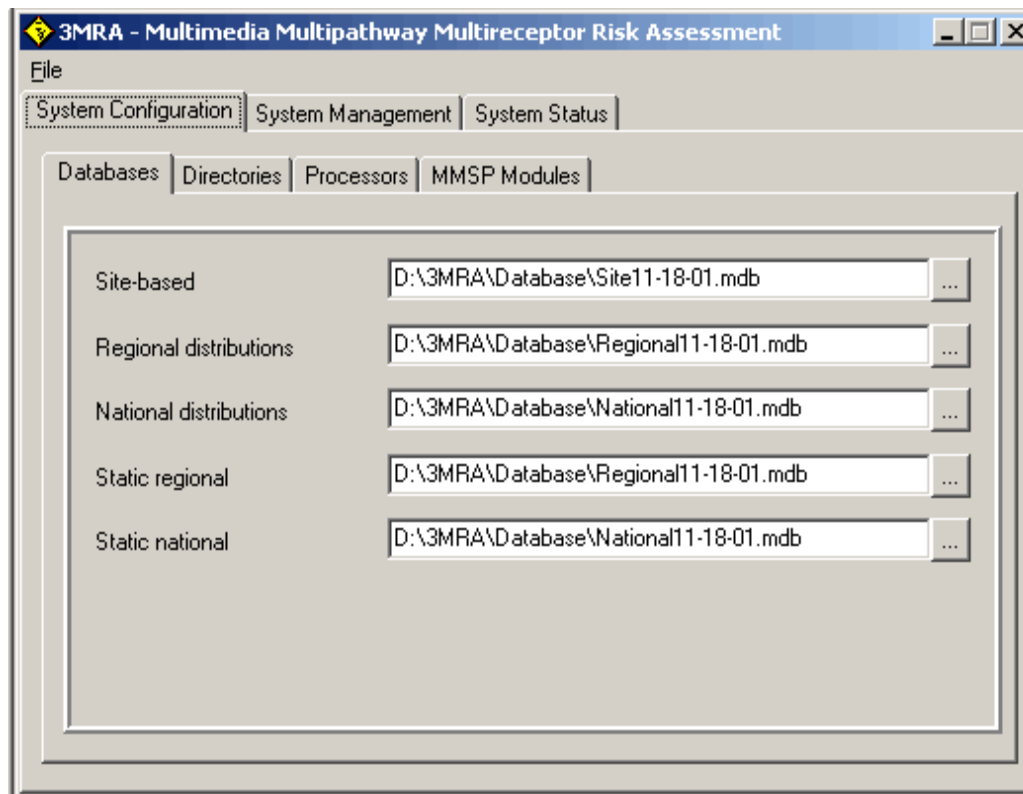


Figure 4.30 3MRA SUI : System Configuration Screen

Directories SubScreen

The Directories subscreen (Figure 4.31) of the SYSTEM CONFIGURATION SCREEN requires the user to input the Directory location specifying where various sets of data files reside. The system data files that need to be defined are illustrated in Figure 4.31 and are as follows:

- Site Simulation Files (SSF)
- Global Results Files (GRF)
- Risk Summary Output Files (RSOF)
- Protection Summary Output Files (PSOF)
- Permanent Storage
- Chemical Properties Database
- Meteorological Database

The data files contained in the SSF, GRF, RSOF, and PSOF are produced by the system during a simulation. The SSF directory contains all input data for the science modules that is extracted from the Site/Regional/National databases and prepared in SSF format for module

consumption. The GRF directory contains all the module output files, each being a unique GRF file. Also contained in both the SSF and GRF directories are the DICTIONARY files that correspond to each science module input file (SSF) and output file (GRF). The RSOF directory contains the Risk Summary Output Files generated by the ELP I. The PSOF directory contains the Protective Summary Output files generated by the ELP II. The Permanent Storage directory contains an archive of all SSF and GRF files resulting from a simulation. These files are saved only if the user specifies a maximum storage option (discussed below). It is typically the case that the storage option is used only in the case of a single site assessment. Storing all SSF and GRF files for a national scale assessment is not possible with current memory limits on the Personal Computers (it would require on the order of several gigabytes for the minimum national assessment and terabytes of storage for a national assessment involving multiple chemicals and hundreds of Monte Carlo iterations). The Chemical Properties directory points to the location where all chemical property data is stored. The Meteorological Data directory points to the location where all meteorological data reside.

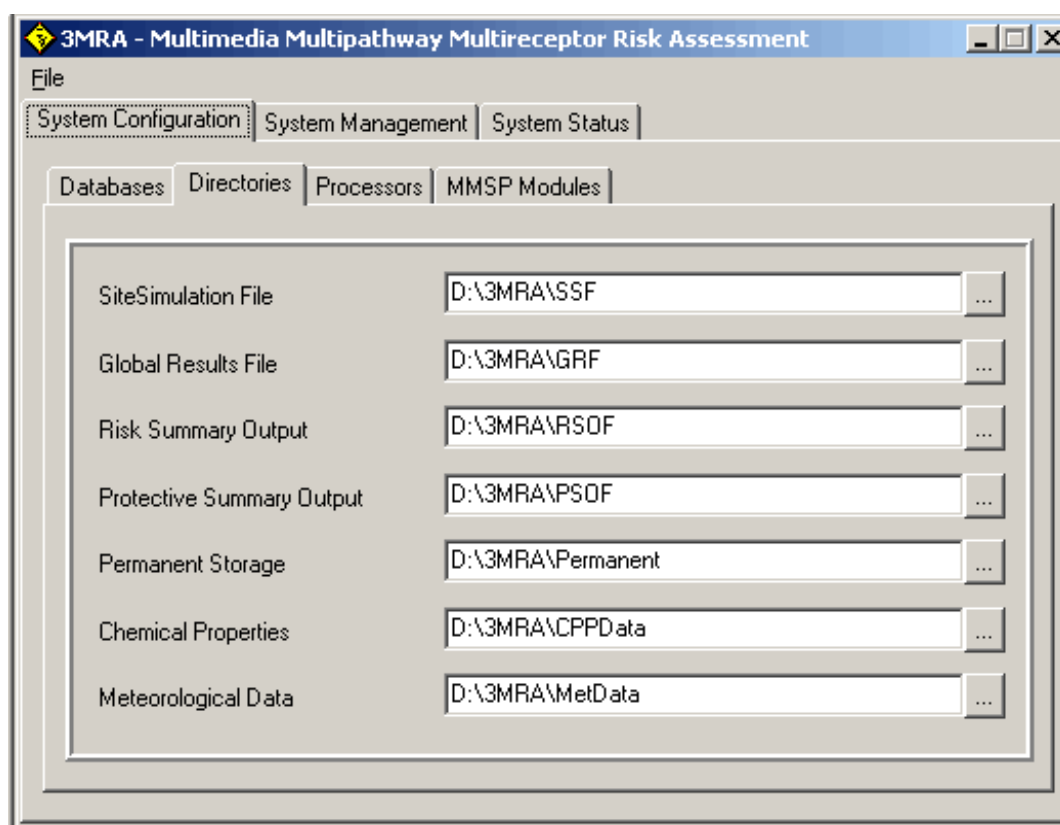


Figure 4.31 3MRA SUI : Directories Configuration Screen

Processors SubScreen

Figure 4.32 displays the Processor subscreen of the System Configuration Screen. A total of six system processors are listed on the screen but only four are implemented at this time.

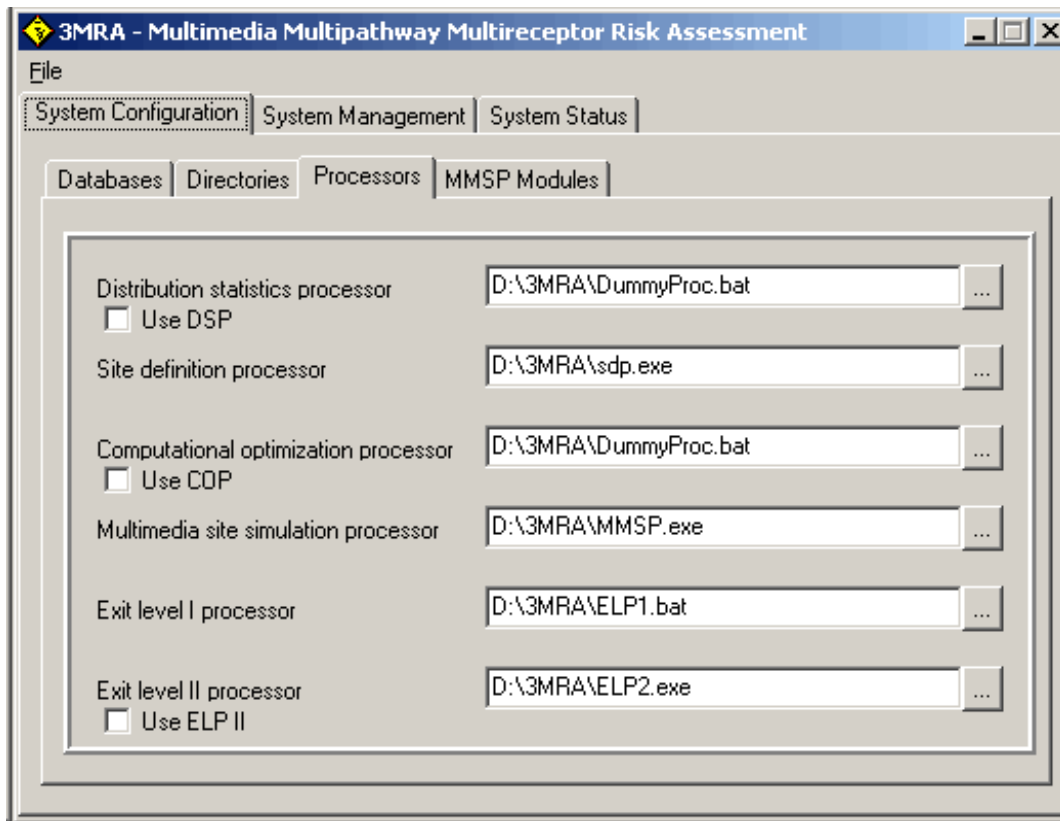


Figure 4.32 3MRA SUI : Processor Configuration Screen

The following table describes the processors and their current implementation status.

PROCESSOR	FUNCTION	STATUS
Distribution Statistics Processors (DSP)	Facilitates Second Stage Monte Carlo Sampling and Simulation	To be implemented in a future version.
Site Definition Processor (SDP)	Transfers site data from Databases to Site Simulation Files	Implemented
Computational Optimization Processor (COP)	Facilitates optimization of simulations.	To be implemented in a future version.
Multimedia Multipathway Simulation Processor (MMSP)	Manages the execution of 3MRA science modules.	Implemented
Exit Level Processor I (ELP I)	Transforms and stores human and ecological risk data.	Implemented
Exit Level Processor II (ELP II)	Develops tabular and graphical representations of exemption levels based on user requests.	Implemented (However, the ELP II is not invoked through this SUI).

The screen includes three small textboxes to the left of the DSP, COP, and the ELP II. These boxes are checked IF the processor is active (which they are not at this point in time). For the DSP and COP the textboxes specifying the file locations are filled with a filename of “DummyProc.bat”. This filename signals to the system that the processor is not active. The SDP, MMSP, and the ELP I must be specified by the user. The ELP II must be specified on this screen even though it is not invoked during a simulation (this is simply an item which has not yet been removed from the screens).

The MMSP Modules SubScreen

The MMSP Modules subscreen is linked to four lower level subscreens, each subscreen collecting directory information about a group of science modules. The four groups of modules specified by the user to run simulations are the source, transport, food chain, and exposure/risk modules. The user clicks on the MMSP MODULES subscreen to specify these module data. Figure 4.33 illustrates the source subscreen. Directory locations and file names for the executable file representing each of the five source types included in the MMSP are specified here. Similar screens are included for the transport, food chain, and exposure/risk modules.

4.2.3 System Management

The functions of the SYSTEM MANAGEMENT SCREEN allow the user to define the sites, chemicals, source types, and waste levels for simulation. It also allows the user to select the level of storage for MMSP modules input (SSF) and output (GRF) files, the mode of operation, the number of Monte Carlo iterations, and seed value for the statistical analysis of the simulation. Each of these functions is accessed by the user through subscreens associated with the SYSTEM MANAGEMENT SCREEN. These functions are described in the following subsections.

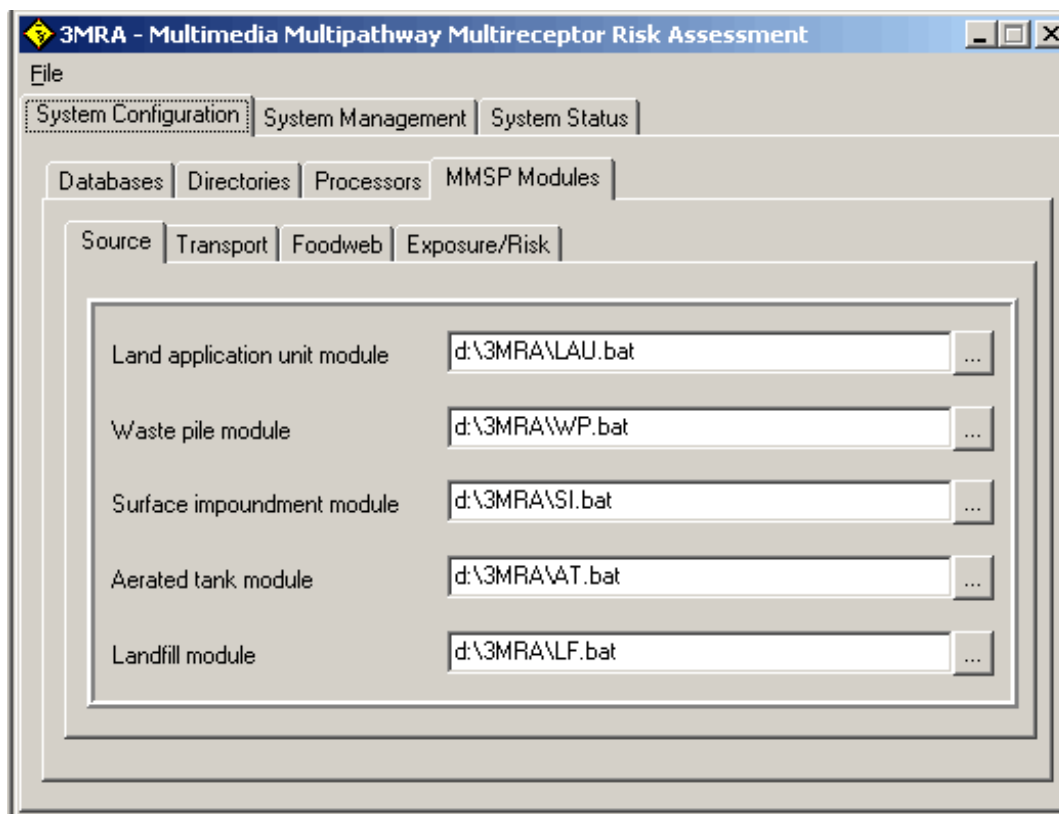


Figure 4.33 3MRA SUI : MMSP Configuration Screen

Selections SubScreen

The SELECTIONS subscreen (Figure 4.34) of the SYSTEM MANAGEMENT SCREEN allows the user to select the sites, chemicals, source types, and waste levels used for the simulation. The user can select a single, subset, or all of the sites, chemicals, source types, and waste levels to be simulated. The sites appear on the subscreen as site identification names that come directly from the Site-Based Database. The chemicals also appear on the subscreen as the actual names defined in the Chemical Properties Database.

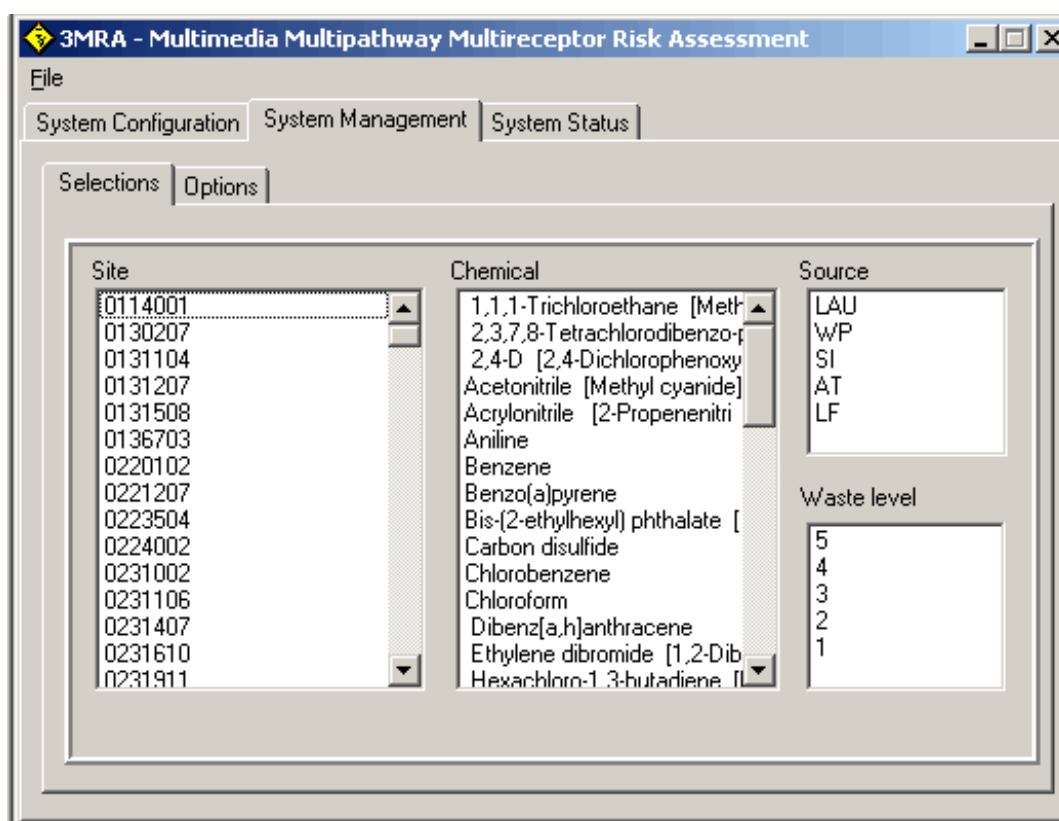


Figure 4.34 3MRA SUI : System Management Selections Screen

The five source types are land application unit (LAU), waste pile (WP), surface impoundment (SI), aerated tank (AT), or landfill (LF). The waste level categories define the waste concentration in wastestreams entering the source. The selection of multiple entities (e.g., sites) is facilitated by two options. By holding down the **Ctrl** key and left clicking on individual selections, each selection will be highlighted, thus, including it as part of the simulation. If the user wishes to highlight a consecutive series of entities (e.g., all chemicals from Benzene through Chloroform) the first entry (Benzene) is left clicked, and while holding down the **Shift** key, left click on the last chemical in the list (Chloroform). To select all available entries of a list the user left clicks on the first entry, scrolls down to the bottom of the list and, while holding down the **Shift** key, left clicks on the last entry.

Options

When the site, chemicals, source types, and waste levels are selected, the OPTIONS subscreen (Figure 4.35) of the SYSTEM MANAGEMENT SCREEN is used to select the data storage level, mode of operation, number of iterations, and seed value used as part of the probabilistic simulation. The storage level selections are currently *minimum* or *maximum*. The minimum storage level keeps only the RSOF files from the simulation while the maximum storage level stores all SSF, GRF, and RSOF files created during the simulation. The number of Monte Carlo iterations (or realizations) for the simulation is defined by the user. The seed value is used by the statistical component of the simulation. This value defines the random sampling seed required for the simulation. If the user needs to duplicate a simulation, this value must be the same as the one used in the original simulation.

The user can select one of three different operation modes for the simulation. The **Debug** mode stops the simulation after every change in iteration, chemical, source type, and waste level. The **Stop on Error** mode stops the simulation only if an error occurs in a processor or module when production runs are being implemented (if the Stop on Error is not selected the simulation simply logs the error and executes the next site simulation). The **Stop on Warning** mode stops the simulation if a warning appears in a processor or module. The **Debug**, **Stop on Error**, and **Stop on Warning** modes can be selected simultaneously by the user. These options are generally utilized only when testing the software of the modeling system. The **Comment box** on this subscreen allows the user to provide descriptive information about the current simulation.

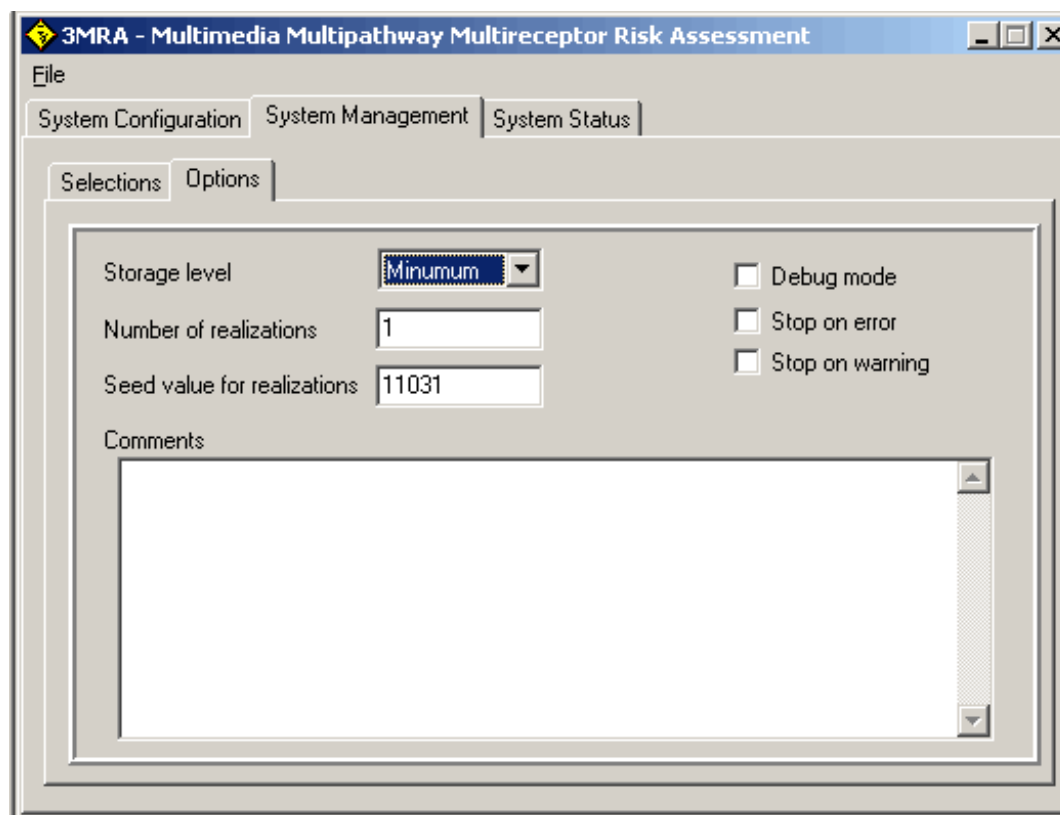


Figure 4.35 3MRA SUI : System Management Options Screen

4.2.4 System Status

The main function of the SYSTEM STATUS SCREEN (Figure 4.36) is to allow the user to follow the progress of the simulation, as it steps through the iterations, sites, chemicals, source types, and waste levels. Depending on the mode of operation the user selected for the simulation (see the OPTIONS subscreen of the SYSTEM MANAGEMENT SCREEN, Section 4.2.2), this screen behaves differently. If the **Debug** mode is selected, the simulation stops after each step whether it is an iteration, site, chemical, source type, or waste level. The user can then select the **Resume** button to continue the simulation or evaluate the results of the simulation (e.g., switch out of the 3MRA modeling system to some other software). If the **Stop on Error** or **Stop on Warning** mode is selected, the software continuously cycles through the simulation until it encounters an error or warning from a processor or module. If an error or warning occurs, the simulation is suspended. The user can evaluate the situation and decide whether to continue the simulation or stop it. If the simulation is not completed, all files created before the suspension of the simulation are stored in the specified locations and are available for future evaluation. If the simulation is suspended, the user can attempt to correct the problem, and then **Resume** the simulation.

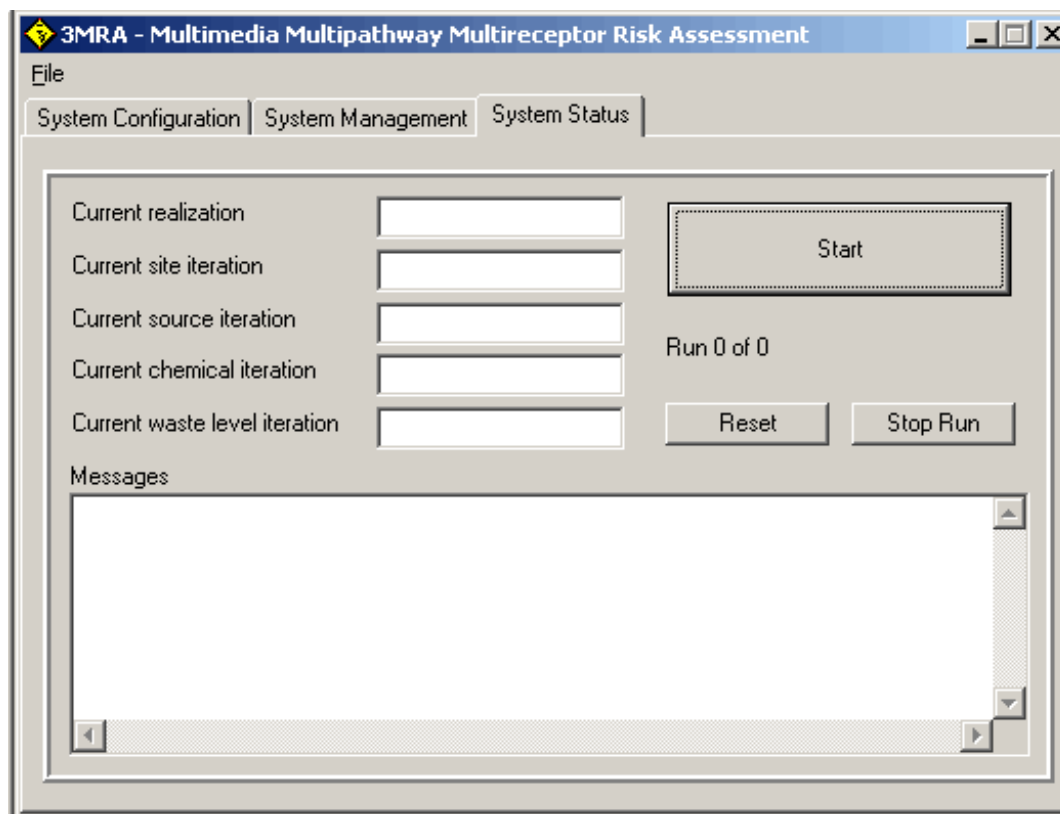


Figure 4.36 3MRA SUI : System Status Screen

Any error or warning message generated by a processor or module is displayed in the message box provided at the bottom of the SYSTEM STATUS SCREEN. These messages help the user determine the status of the simulation and whether to continue or suspend the simulation. Error and warning files that correspond to these messages are created by the system. The user can utilize these files to determine the problem and continue the simulation, or stop it and correct the problem. If the user stops the simulation and corrects the problem, the simulation can be set up where it stopped and the simulation resumed using the **Resume** button.

4.3 Post Simulation Analysis

This section covers the tools used for post simulation analysis. Section 4.3.1 describes the tools available to review and analyze results of national assessments. These tools include the Exit Level II Processor (ELP-II) and the Risk Visualization Processor (RVP). Section 4.3.2 describes the Site Visualization Tool (SVT) that facilitates visual review and analysis of single site assessments.

Example datasets for both a national assessment and site assessment have been provided in the installation of the 3MRA modeling system. The essential features of the analysis tools described by applying them to the review of two sets of example results.

4.3.1 Analysis of National Assessment Results (ELP II/RVP)

At the completion of a national assessment simulation there exists the Risk Summary Output Files (RSOF). The RSOFs are Microsoft Access databases. The RSOFs can be directly viewed by using Microsoft Access software. The RSOFs are input to the ELP II for the purpose of exploring the relationship between waste concentration levels (Cw's) and the national probabilities of risk protectiveness. The ELP II provides a user interface that allows the graphical exploration of the risk summary data as well as the ability to generate Protective Summary Output Files (PSOFs) that provide tables of national exemption levels based on data contained in the RSOFs and regulatory criteria established by the user.

Let's execute an example of a national assessment and use the ELP II and the RVP to review risk/hazard results and generate national exemption levels. For this example a national exemption level will be determined for benzene. Figure 4.37 illustrates the **Selection Subscreen** of the SUI **System Management tab** needed to communicate the national assessment to the 3MRA modeling system. Notice that all sites are selected, only the chemical benzene, all waste management units, and all five wastestream concentration levels.

With the selections made the user proceeds to the **Options Subscreen** of the SUI **System Management tab** and specifies "Minimum" storage, one Monte Carlo realization, leaves the default random number seed as 11031, and leaves the options related to debug, error, and warning modes unchecked. The user then enters the SUI **System Status Subscreen** and presses the **Start button**. The execution of this national assessment for benzene takes on the order of two full days to complete the 2095 individual site simulations (on a P III 1.0GHz PC).

NOTE : The C:\ is used here as an example of the directory location where the 3MRA modeling system has been installed. The drive specification must correspond to the one specified by the user during installation.

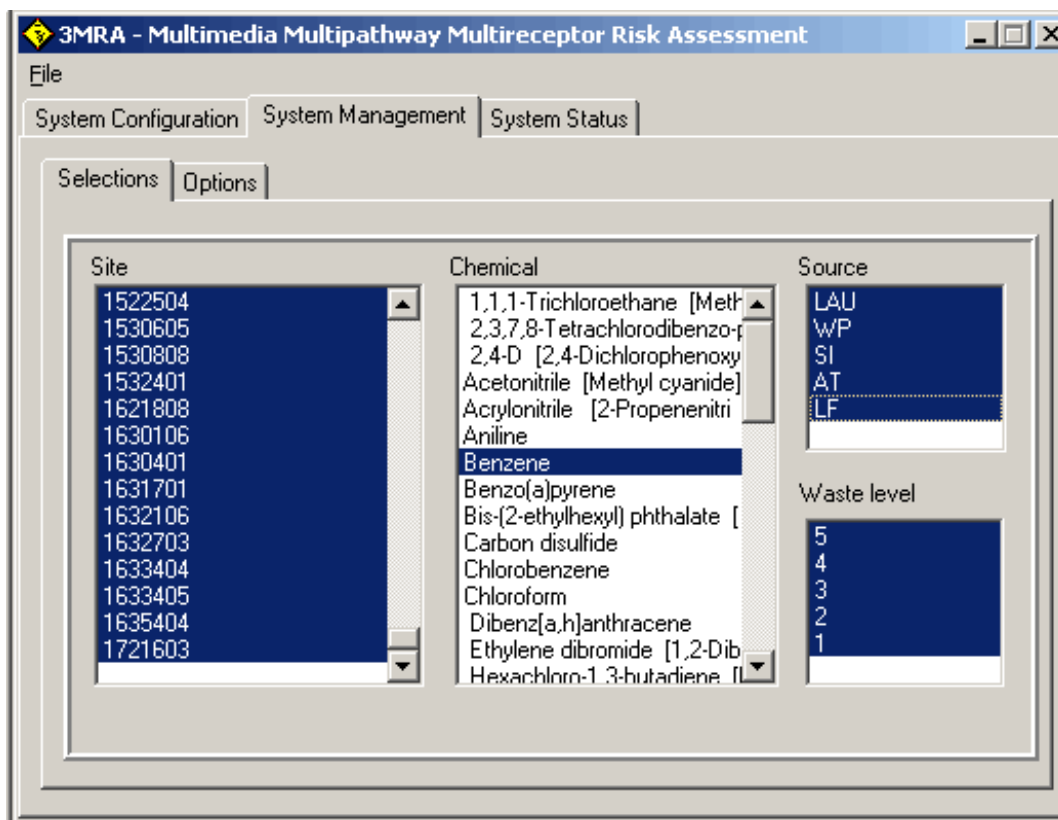



Figure 4.37 3MRA SUI : Selection Screen for National Assessment of Benzene

To facilitate the objective of demonstrating the ELP II/RVP the user has been provided the header file and RSOFs that result from this assessment. Upon installation of the 3MRA modeling system the example RSOF is located in the subdirectory C:\3MRA\ExampleOutput\RSOF.

Before this set RSOF databases can be accessed by the ELP II, the contents of the directory must be copied to the standard RSOF directory (i.e., C:\3MRA\RSOF). This is facilitated by providing the batch file named “MoveFiles.bat” in the C:\3MRA\ExampleOutput directory. The user simply double clicks on the “MoveFiles.bat”, the batch file executes transferring the example RSOF databases to the C:\3MRA\RSOF directory, where the ELP II expects to find them. The header file is located in the C:\3MRA\SSF directory under the name “hdprdex1.ssf”.

To start the ELP-II, the user selects the Windows Start button and clicks PROGRAMS/3MRA/ELPII. Figure 4.38 illustrates the initial screen that appears upon the invocation of the ELP II. The user then goes to the menu and selects **File** and then **Open**, which accesses the Explorer window for the purpose of locating the appropriate “header file” that was used to generate the national simulation results. The user locates and highlights the appropriate “header file” as C:\3MRA\SSF\hdprdex1.ssf and clicks on the OPEN button.

The user then left clicks on the  button to display the list of chemicals, selecting benzene for this example (only benzene is available even though other chemicals are listed). Similarly, the user selects from among the WMU source options (e.g., Landfill). Upon selection of the chemical and source type the screen shown in Figure 4.39 is displayed. The screen displays a list of all factors and options associated with 1) establishing the quantitative

relationship between C_w and Probability of Protection (i.e., the percentage of sites that protect a specified percentage of receptors at a specified risk/hazard level, e.g., a human carcinogenic risk of 10^{-6}), and 2) computing national exemption/exit levels.

There are three type of C_w vs Probability of Protection relationships that can be generated, each a function of a different measure of risk (i.e., human carcinogenic risk, human hazard, and ecological hazard). Not all chemicals present all three types of risk and also, effects data may not be available for any given chemical for any given risk measure. Thus, depending on the selections made the ELP II may simply inform the user of its inability to develop certain C_w vs Probability of Protection relationships.

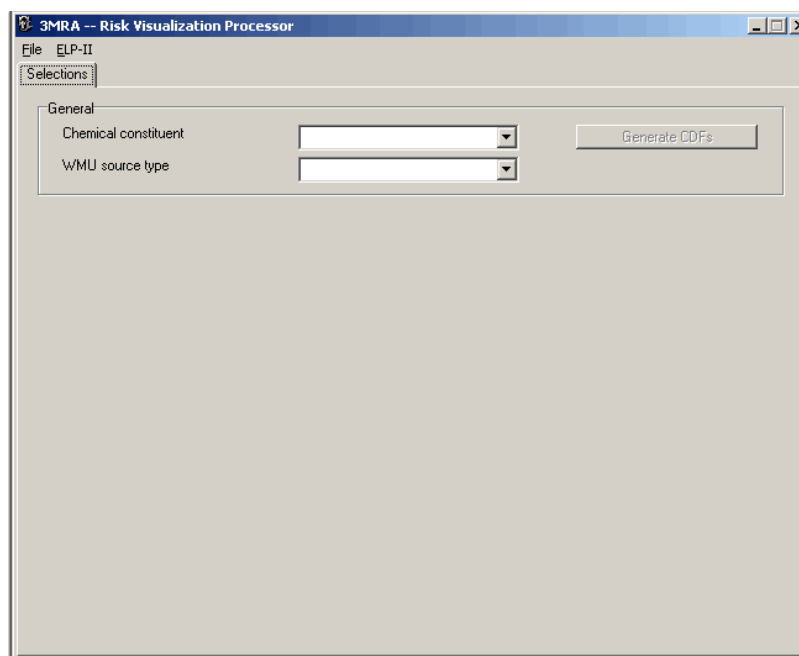


Figure 4.38 Initial ELP-II Screen

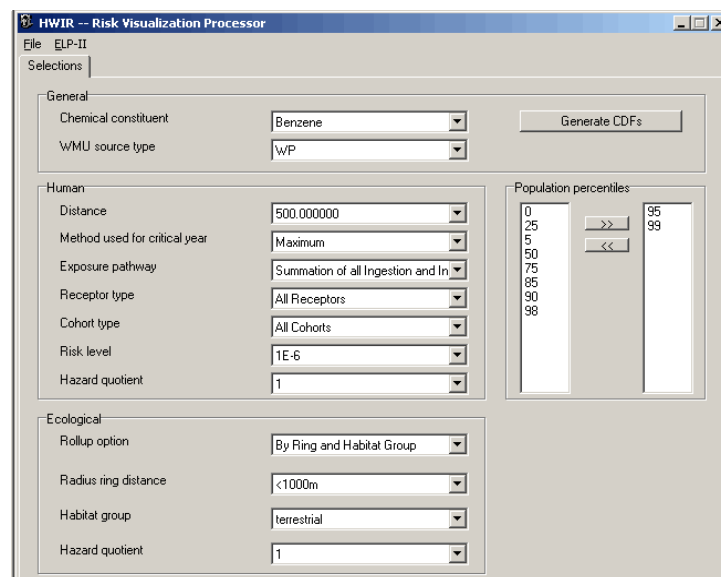





Figure 4.39 ELP II Options Screen

The ELP II presents the user with default selections for each regulatory factor. The user can modify the selection for any factor by left clicking the  button and making an appropriate selection. On the right hand portion of the screen the user selects the population percentiles for which the Cw vs Probability of Protection relationship should be generated. The options are listed in the left textbox (i.e., 0, 5, 25, 50, 75, 85, 90, 95, 98, 99). The user highlights the percentages of interest and clicks the  button to transfer the percentage to the right hand textbox where it becomes part of the ELP II/RVP processing. Removing the percentages from the right hand textbox is accomplished in a similar fashion using the  button.

Given the selections the user then clicks the **Generate CDFs** button. Because benzene poses a carcinogenic risk and not other health hazards a message box with the message 'No table available for human hazard quotient summary' is displayed. Figure 4.40 shows the Human Risk screen after the button has been clicked. This screen has three functions. First, in addition to the **Selection tab** there is a tab for each risk measure selected by the user, allowing the user to view the various Cw vs Probability of Protection graph. Secondly, it displays the relationship between Cw and Probability of Protection. A curve is included for each population percentile selected by the user. Notice that as Cw increases the Probability of Protection either remains the same or decreases. In this example, for instance, the graph shows there is an 80 percent probability that any given site is protective of 95 percent of all receptors located at the site at a risk level of $1e-6$ and a Cw of $1e3$ ug/g. Or, said a bit differently, that 80 percent of the sites are protective of 95 percent of the receptors located at individual sites at the site at a risk level of $1e-6$ and a Cw of $1e3$ ug/g. The third function of the screen is to facilitate the computation of interpolated values for exemption levels (shown as interpolated Cw). The user specifies a population percentile and Probability of protection in the text windows at the top of the screen and the ELP II computes a value for the corresponding Cw (interpolated between plotted points if necessary).

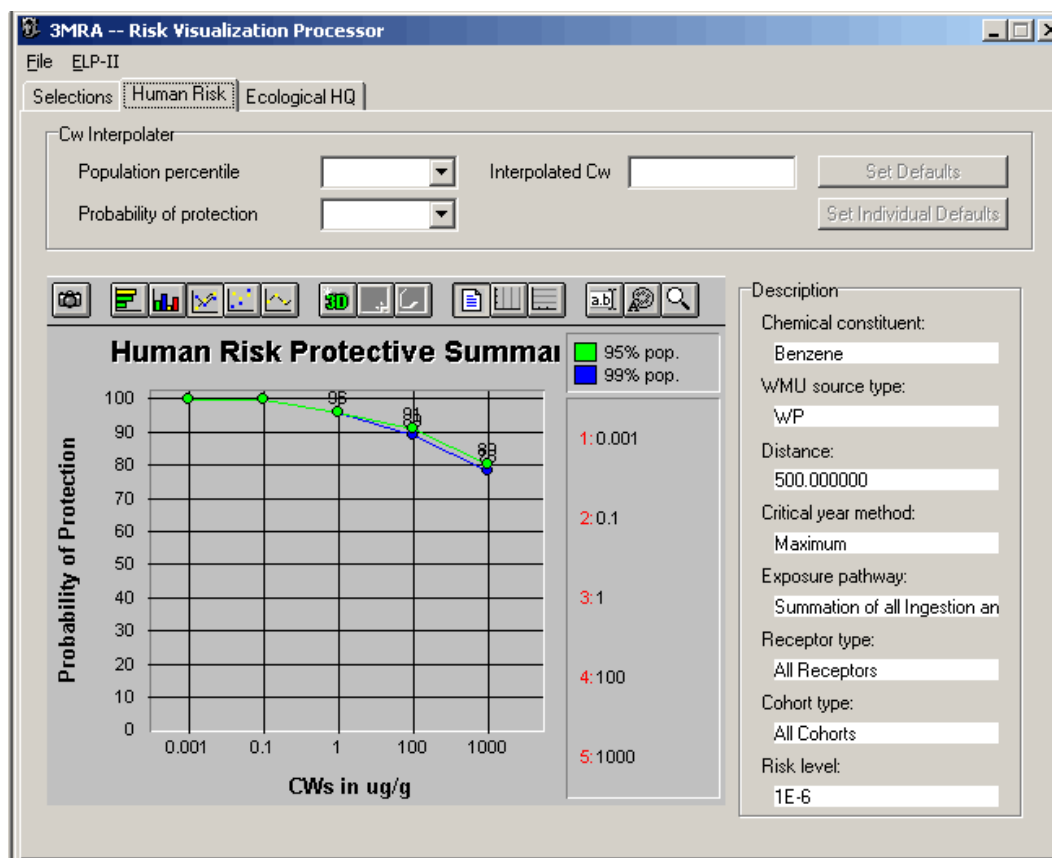


Figure 4.40 ELP II Human Risk Protective Summary Screen

These values of Cw represent possible exemption levels that may, for example, define the threshold between hazardous and non-hazardous waste. The user can return to the selection screen and modify various regulatory factors and develop new plots. This interaction between the user and the RSOE database can be fully explored via the ELP II/RVP.

Figure 4.41 Shows the Ecological Hazard Quotient screen. Notice that in this graph all sites are protective of all terrestrial receptors, even at the highest possible Cw. Thus, from this graph one would conclude that under no scenario does benzene pose a risk to terrestrial receptors (keep in mind this is a hypothetical graph for illustrative purposes only).

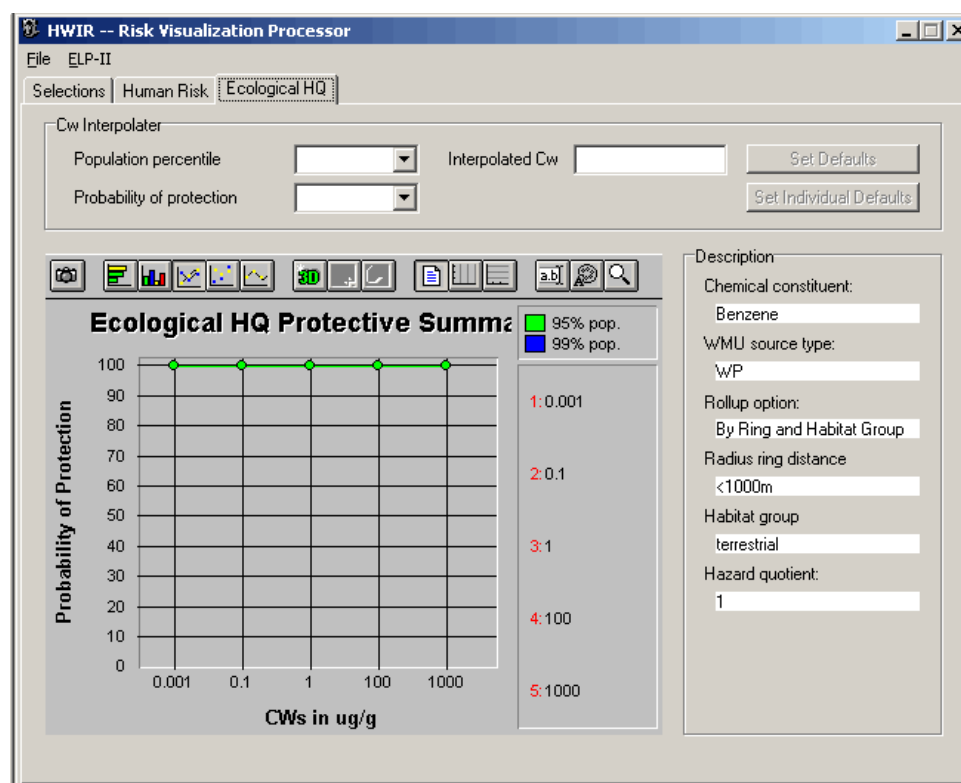


Figure 4.41 ELP II Ecological HQ Protective Summary Screen

The user, via this graphical plotting capability, is free to explore the possibilities regarding the relationship between Cw and Probability of Protection. Additionally, the user can specify a population percentile and probability of protection (i.e., percentage of sites protective at the given population percentile) and have the ELP II compute an interpolated value of the exemption level (Cw). This functionality appears at the top of Figures 4.40 and 4.41 within the box labeled Cw Interpolator.

The ELP II also allows the user to generate output tables containing exemption levels under varying conditions (as described in Section 3.3.9.2). Figure 4.42 illustrates the options that will appear when the ELP II tab is invoked. The tables are stored in comma separated data files contained in C:\3MRA\PSOF. The files are easily read into a spreadsheet such as Microsoft Excel.

4.3.2 Analysis of Site Assessment Results

While the 3MRA modeling system is designed principally to execute national assessments it is also capable of singling out a specific combination of site, chemical, WMU, and Cw for simulation. This capability has been particularly useful during the verification testing of the 3MRA modeling system. It is also important in the context of comparing results of the 3MRA with other modeling systems designed for similar purposes. To demonstrate the application of the 3MRA to a single site and show how detailed results of a site application can be reviewed visually we will use an example. Outputs for this example are provided in the installation of 3MRA.

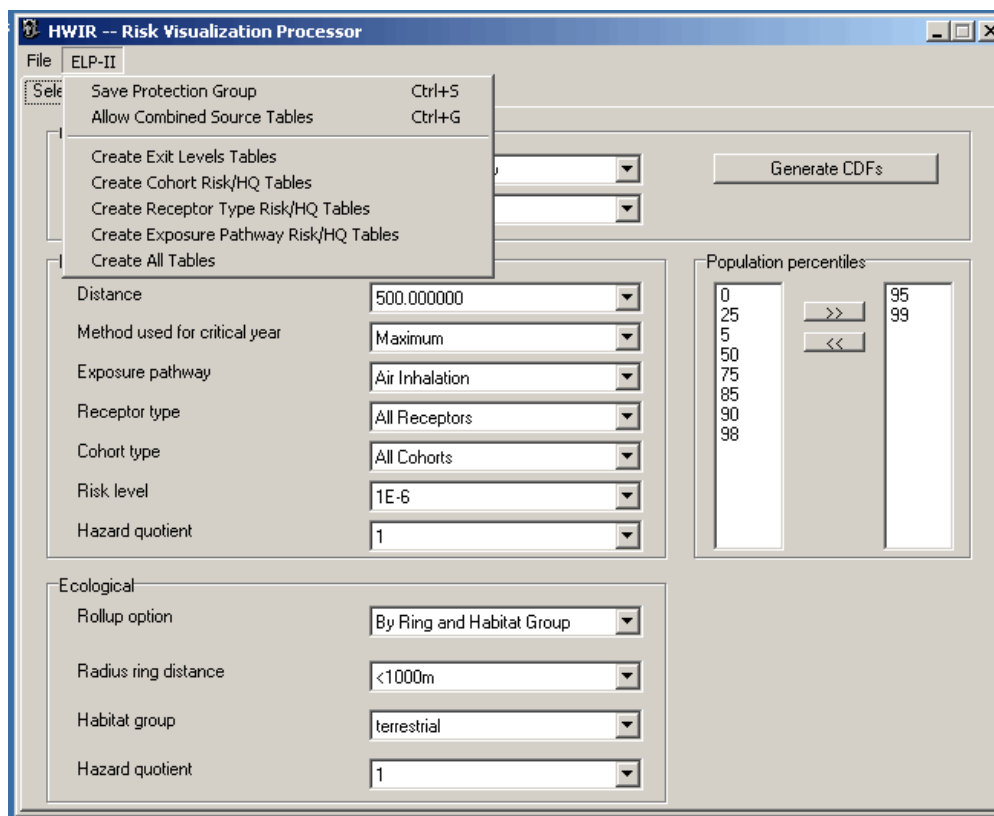


Figure 4.42 ELP II Tabular Output Selection Screen

Figure 4.43 illustrates the **Selection Subscreen** of the **SUI System Management tab** needed to communicate the single site application to the 3MRA modeling system. Notice that one site is selected (ID# 0114001) one chemical (CAS ID 71-55-6), one waste management units (WastePile, WP), and one wastestream concentration level (4). All other SUI input screens should be populated as described in Section 4.2.

With the selections made, the user proceeds to the **Options Subscreen** of the **SUI System Management tab** and specifies “Maximum” storage, one Monte Carlo realization, leaves the default random number seed as 11031, and leaves the options related to debug, error, and warning modes unchecked. The user then enters the **SUI System Status Subscreen** and presses the **Start button**. The execution of this site assessment for benzene takes on the order of a few minutes to complete (on a P III 1.0GHz PC).

Selecting Maximum storage causes the modeling system to save all SSF and GRF files generated during the simulation. Because only one site is executed there will be one set of SSF and GRF files generated in this example. The SSF and GRF files are saved under the C:\3MRA\Permanent directory. For this example the SSF and GRF files have been placed under the C:\3MRA\ExampleOutput directory. To continue to follow this example the user must either execute the simulation or copy the SSF and GRF files from the ExampleOutput subdirectory into the C:\3MRA\Permanent\SSF and C:\3MRA\Permanent\GRF directories. If the user elects to execute this site assessment the resulting SSF and GRF files will be placed in the C:\3MRA\Permanent directory.

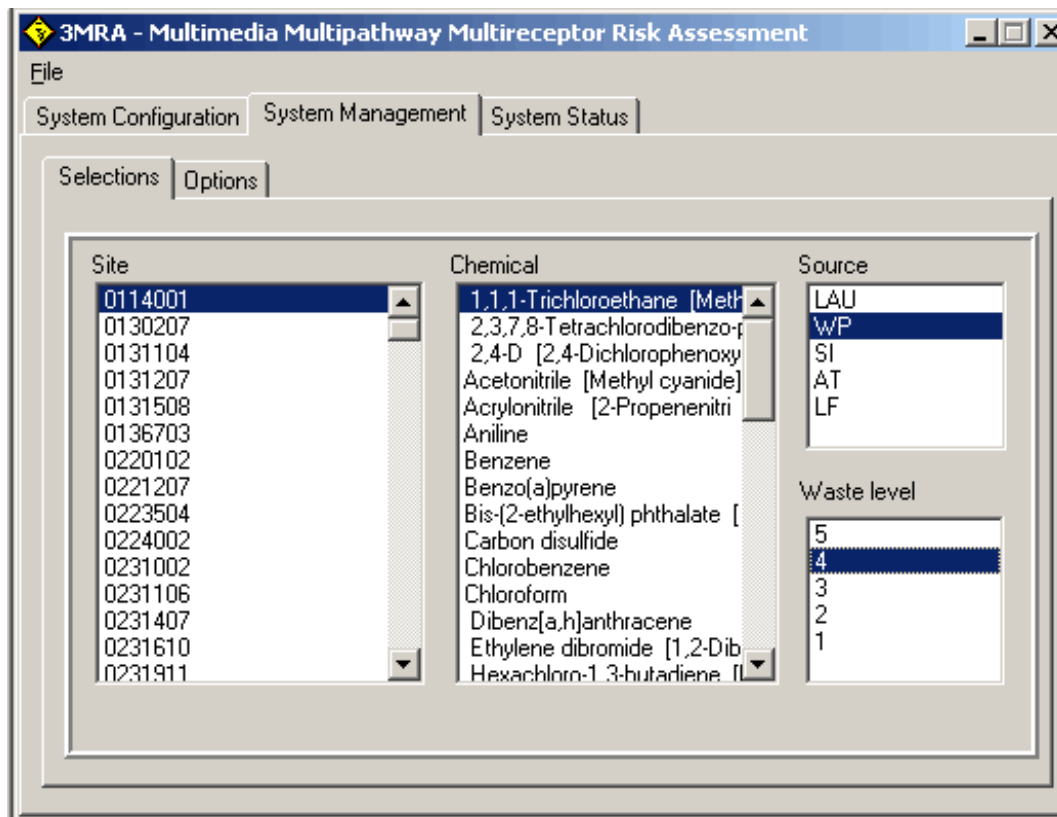


Figure 4.43 3MRA Selection Screen for Site Example

4.3.2.1 Site Visualization Tool (SVT)

The purpose to the Site Visualization Tool is to allow the user to view a complete set of science module results from a single site simulation. Each of the 3MRA science modules produces a key set of results in the context of a multimedia risk assessment. For example, each of the source modules estimates time series releases of contaminant to air, groundwater, watershed, and surface water. Each of these time series is input to a medium-specific fate and transport module with the result being a time series of medium concentrations at human and ecological exposure locations. From here, the foodweb modules estimate future concentrations of contaminant within various trophic levels. Finally, the exposure and risk modules generate estimates of the time series of exposure and risk. The SVT is designed to read each of the Global Output Files (GRFs) generated during the execution of a site and display all the time series results

for simultaneous viewing via an HTML plotting format. When viewed in this fashion the user can identify trends within and across time series.

There are several important uses of this graphical tool. First, with respect to Quality Assurance the SVT provides an efficient means by which to identify anomalies in the results generated by the science modules.

The SVT is a Java based application that requires the Java runtime environment to be installed for the SVT to work.. This runtime environment is installed during the 3MRA installation as described in Section 4.1. The SVT is currently Beta version software. This means that the software is fully functional but has not undergone final review, testing, and documentation.

To launch the SVT, the user selects the Windows Start PROGRAMS/3MRA/SVT. Figure 4.44 displays the SVT user interface. To execute, the SVT must receive the 3MRA “header file” name associated with the site simulation, the location of the SSF and GRF files that resulted from simulation, and the directory location for storing the graphical output files generated by the SVT. The SSF, GRF directory specifies the parent folder in which the SSF and GRF folders are located. For this example the SSF, GRF directory is D:\3MRA\ExampleOutputs\Permanent\WP011400171-55-6Cw4R1. The header file specifies which header file the user would like to use for the SVT analysis. For this example, the header file name and location is D:\3MRA\ExampleOutputs\Permanent\WP011400171-55-6Cw4R1\ssf\hdprod.ssf. The output directory specifies where the generated output graphics will be placed. For this example the results should be D:\3MRA\ExampleOutputs\Permanent\WP011400171-55-6Cw4R1.

The status label on the bottom of the window informs the user of the current SVT status.

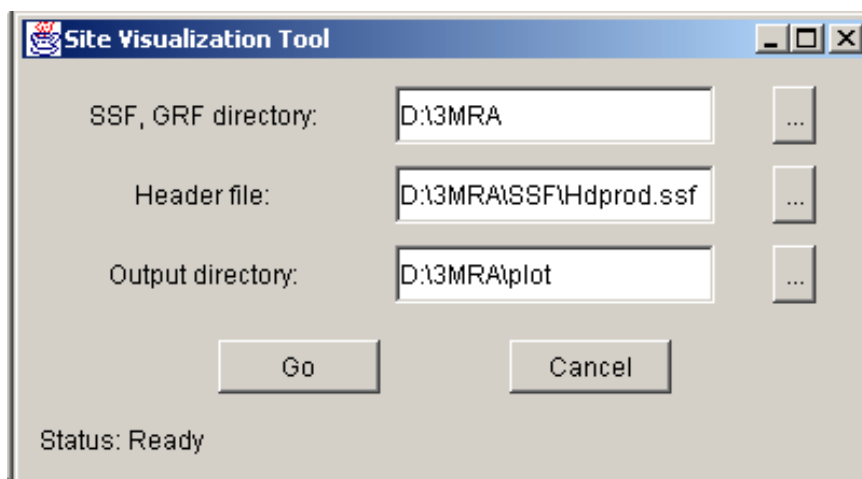


Figure 4.44 SVT User Interface Screen

Once the required information has been correctly entered, the user clicks the **Go** button. Alternatively, if the user does not wish to proceed, the clicking the **Cancel** button will end the SVT application. When the SVT has finished processing, the Status bar will display: ‘Status: Done!’. The output of the SVT is a collection of graphics illustrating various time-varying characteristics of the specified site. To view the SVT output, the user should open the index.html file located in the folder indicated by the ‘Output directory:’ box on the initial SVT screen. Double-clicking on the index.html file will open the file in the default Internet Browser (e.g.

Internet Explorer, Netscape Navigator). Figure 4.45 illustrates an example index.html file. Clicking on an individual graph will bring up the full size image in the browser. For example, clicking on the 'Soil Concentration' graph brings up a full size Soil Concentration image as shown in Figure 4.46.

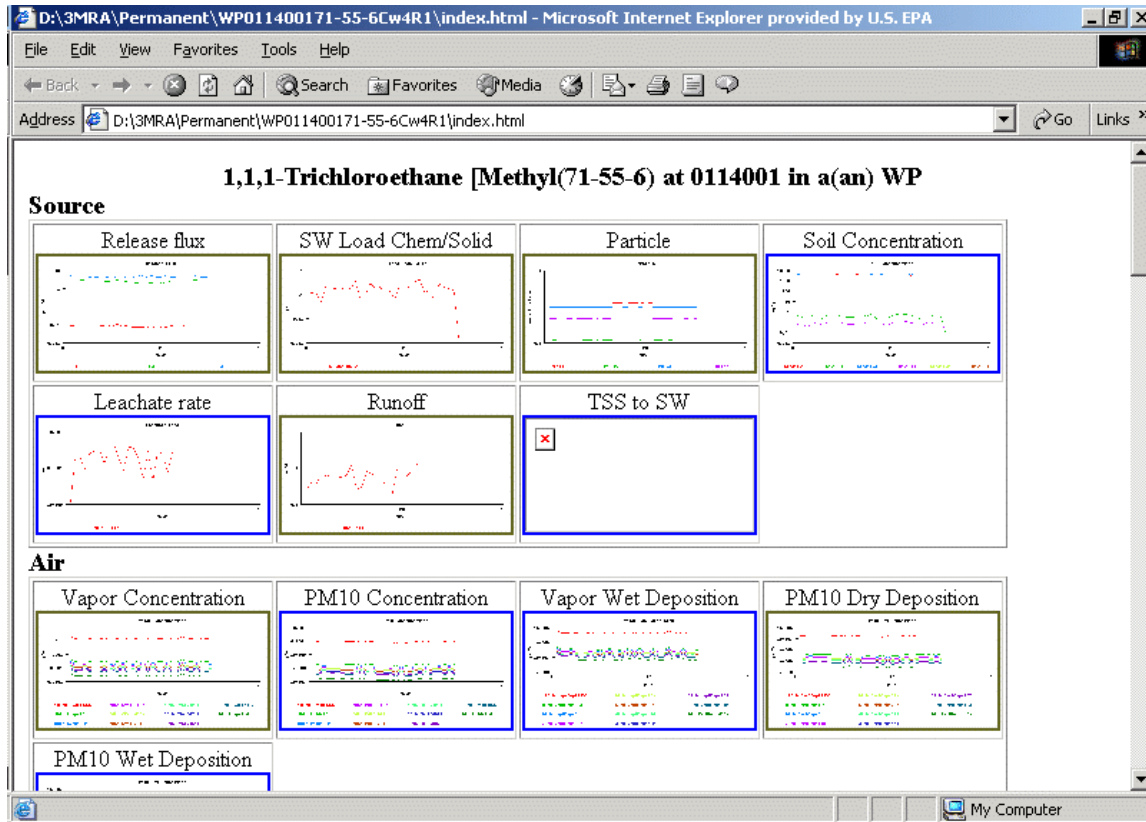


Figure 4.45 Example SVT Output

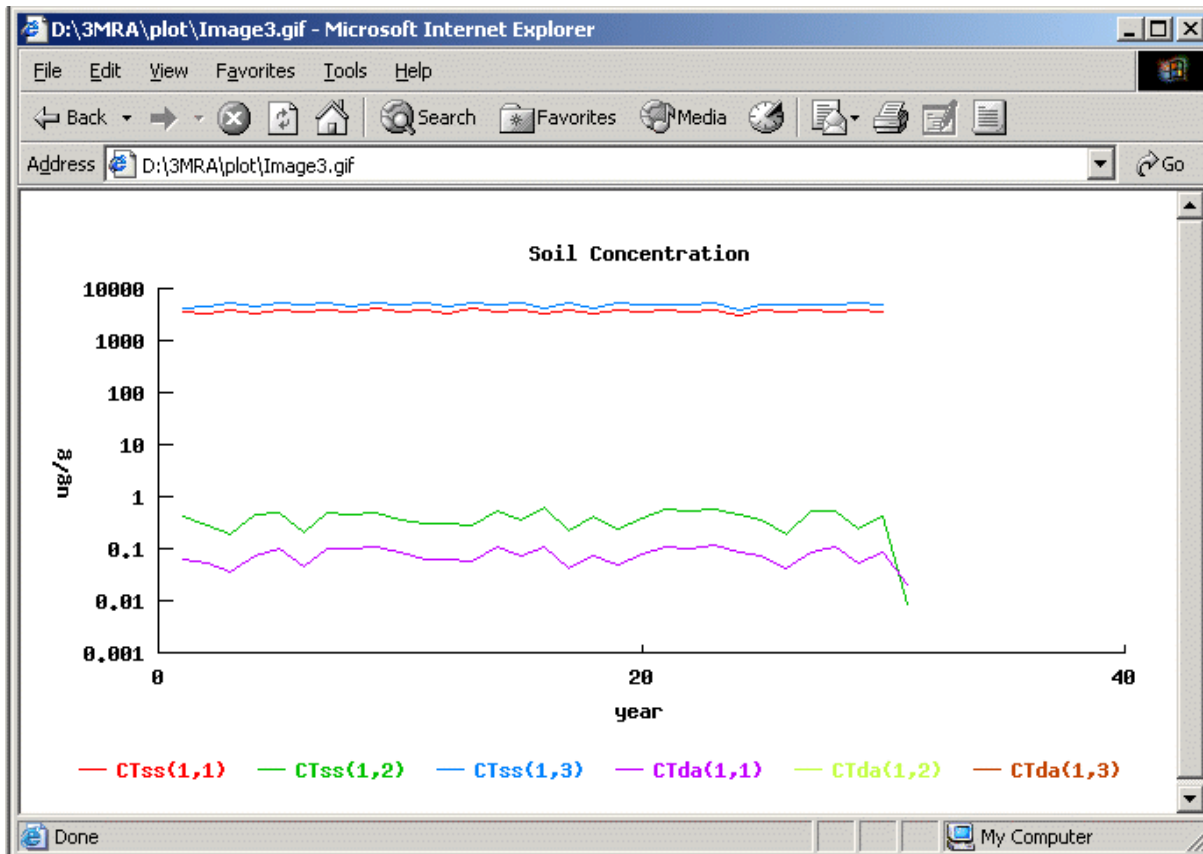


Figure 4.46 Sample SVT Soil Concentration Graph