

US EPA ARCHIVE DOCUMENT

3.0 3MRA Technology

This section describes the integrated 3MRA technology design. The design is presented in three segments. Section 3.1 describes the specific list of system requirements based on the 3MRA methodology. Section 3.2 describes the overall system design and how it reflects the 3MRA methodology and the associated requirements. Section 3.3 presents a more detailed description of the individual components of the modeling system.

3.1 System Requirements

The 3MRA technology design is “requirements-based”, that is, statements of specific functionality along with statements of hardware and software specifications combine to define the requirements that the technology must satisfy. Requirements specify “what” needs to be done but do not dictate “how” the requirement is to be implemented. The collective statement of requirements is transcribed into a software system design and subsequently implemented into a fully functional modeling system.

In laying out the systems level design for the 3MRA technology three categories of requirements are specified. First and foremost, requirements related to the transcription of the 3MRA national assessment methodology into a computer-based technology is presented. These requirements essentially map the functional needs related to the elements of the methodology (national assessment strategy, models, data) to functions required of the technology. Second, there are programmatic requirements that must be met. These requirements reflect the larger EPA regulatory and science research context within which the 3MRA modeling system will be applied, maintained, and enhanced. Finally, there are requirements related to the computer software and hardware environment within which the 3MRA technology is intended to operate and several computer science oriented requirements that target modern software engineering practice.

Section 3.1.1 describes the requirements for transcribing the 3MRA national assessment methodology. Section 3.1.2 describes Agency programmatic requirements and Section 3.1.3 describes the software and hardware requirements .

3.1.1 Transcription of 3MRA Methodology into Technology Requirements

The specific system requirements for transcribing the full 3MRA methodology into a computer software technology are as follows:

SITE-BASED MODELING

- Provide an integrated site scale environmental risk assessment model. The model must simulate physical/chemical/biological processes related to :
 - 1) five waste management unit types,
 - 2) full multi-media fate and transport (i.e., air, watershed, vadose zone, aquifer, and surface water),
 - 3) terrestrial and aquatic foodweb,
 - 4) a farm foodchain,

- 5) human/ecological exposure, and
- 6) human/ecological risk
- Must accommodate legacy models that have long history of use and acceptability (e.g., EXAMS, ISC).
- Provide a software management system capable of executing a science-based model for the purpose of simulating site scale human and ecological risk.

DATA

- Store site-based data for 201 sites that are geographically distributed across the U.S.
- Provide data storage for environmental variables characterized at regional and national scale.
- Accommodate statistical representation for all data contained in site-based, regional, and national databases.
- Provide for the storage of all data required to execute a 3MRA risk assessment at 201 facilities distributed across the U.S.
- Allow statistical sampling of data values for any variable contained in the databases.
- Facilitate statistical sampling from the following distributions : Uniform, Integer Uniform, Triangular, Normal, Lognormal, Transformed Lognormal, Weibull, Empirical, Gamma, SU, SB, Johnson SB, Exponential.
- Provide database of chemical-specific properties (physical/chemical/biological constants/rates/factors).
- Store and access meteorological data on hourly, daily, monthly, and annual average basis for MET stations across the U.S.
- Accommodate “legacy” databases that may be “hardwired” to legacy models.
- Provide for the centralization for all data that may be shared/used by multiple science modules.

NATIONAL ASSESSMENT STRATEGY

- Provide capability to execute nested loops of 3MRA assessments factors, including chemicals, sites, waste management units, wastestream concentration levels, and Monte Carlo iterations.
- Facilitate a two-stage Monte Carlo simulation, the first stage of which is executed for a specified number of sites containing waste management units.
- Establish tiered or prioritized access to databases containing assessment data (Site-based, Regional, and National databases) .
- Manage the execution of site-based risk assessments using 3MRA science models and databases, each simulation will represent a combination of site, chemical, waste management unit, and waste constituent concentration.
- Generate and store risk matrices, i.e., risk estimates as a function of site, monte carlo realization, receptor, receptor cohorts, exposure areas, contact media, exposure pathways, and exposure routes.
- Generate measures of protection for both graphical and tabular display.

3.1.2 Programmatic Requirements

Programmatic requirements for the 3MRA technology design reflect specific constraints and technology extension needs imposed by the EPA Office of Solid Waste and the Office of Research and Development. These requirements are especially important from the perspective of developing a system design. The 3MRA technology design reflects significant consideration of anticipated future applications of the 3MRA methodology and technology to a myriad of regulatory assessments.

These requirements include the following :

- Implement the 3MRA methodology in a manner that is adaptable to a wide range of specific assessments that may use the methodology.
- Initial implementation must be operational within short-term regulatory time frame of OSW.
- Facilitate integrated research by providing a modeling environment within which modelers could develop, assess, and compare models and modeling approaches to addressing environmental problems.
- Must be extensible to allow site-specific assessments in addition to national scale site-based assessments.
- Free modelers from need to develop all peripheral software (e.g., user interfaces, data/model analysis/connectivity tools, etc.).
- Perform modeling based assessments : provide users a modeling technology that provides access to a community of models, data bases, and data analysis tools as well as an ability to “build” assessment strategies.

3.1.3 Software Environment and Software Engineering Requirements

The software related requirements include the specification of the hardware platform and operating systems upon which and within which the 3MRA technology is to operate. In addition, the software engineering requirements include features that accommodate access to and use of the technology by model developers not involved in the original development. The list of software-based requirements for the 3MRA technology include the following :

SOFTWARE/HARDWARE/UTILITIES

- Implement on IBM-compatible personal computers (PC) and be designed to run on a Pentium (586)-compatible computer with a 200 MHZ processing speed, 64 megabytes of RAM, and a 6-gigabyte hard drive or greater. Greater capacity is recommended.
- Operate in and have applications compiled for a MS Windows 98/2000/NT environment (32-bit)
- Be designed with performance criteria emphasizing run-time efficiencies.
- Accommodate a variety of programming languages (i.e., FORTRAN, C++, C, Visual Basic, Java)
- Provide system user interface that facilitates the setup of 3MRA national risk assessments

- Provide for internal data quality assurance with respect to data representation and interchange
- Provide flexible model execution management that allows all or a subset of the full set of multi-media models to be included in an assessment
- Monitor and report Central Processing Unit (CPU) usage per major system component
- Facilitate user access to results and importing them to other applications for additional data analyses.
- Facilitate plug and play features that allow immediate system access of new components (e.g., alternative models of watershed fate and transport)

3.2 System Design

The objective of the 3MRA software technology design is to transcribe the statement of requirements into an integrated system design that clearly establishes functional components and the operational relationship among them. From the statement of requirements we can extract a high level algorithm, or set of steps, that the technology must execute. These steps help define the major segments or components of the software system design with the relative order and sequencing of the steps defining the operational relationship among the components. From here, the design is hierarchical in that each of the principal steps of the algorithm (or components of the system) are expanded to deeper levels of detail, and as they are an overall architecture for the system unfolds. The high level algorithm and the corresponding technology system design are presented in this section. Section 3.3 then presents a more detailed summary of the system components, their specific function and the relationship among them.

Figure 3.1 illustrates the 3MRA national assessment methodology in the form of an algorithm illustrating the highest level functionality that must be accommodated in the system design.

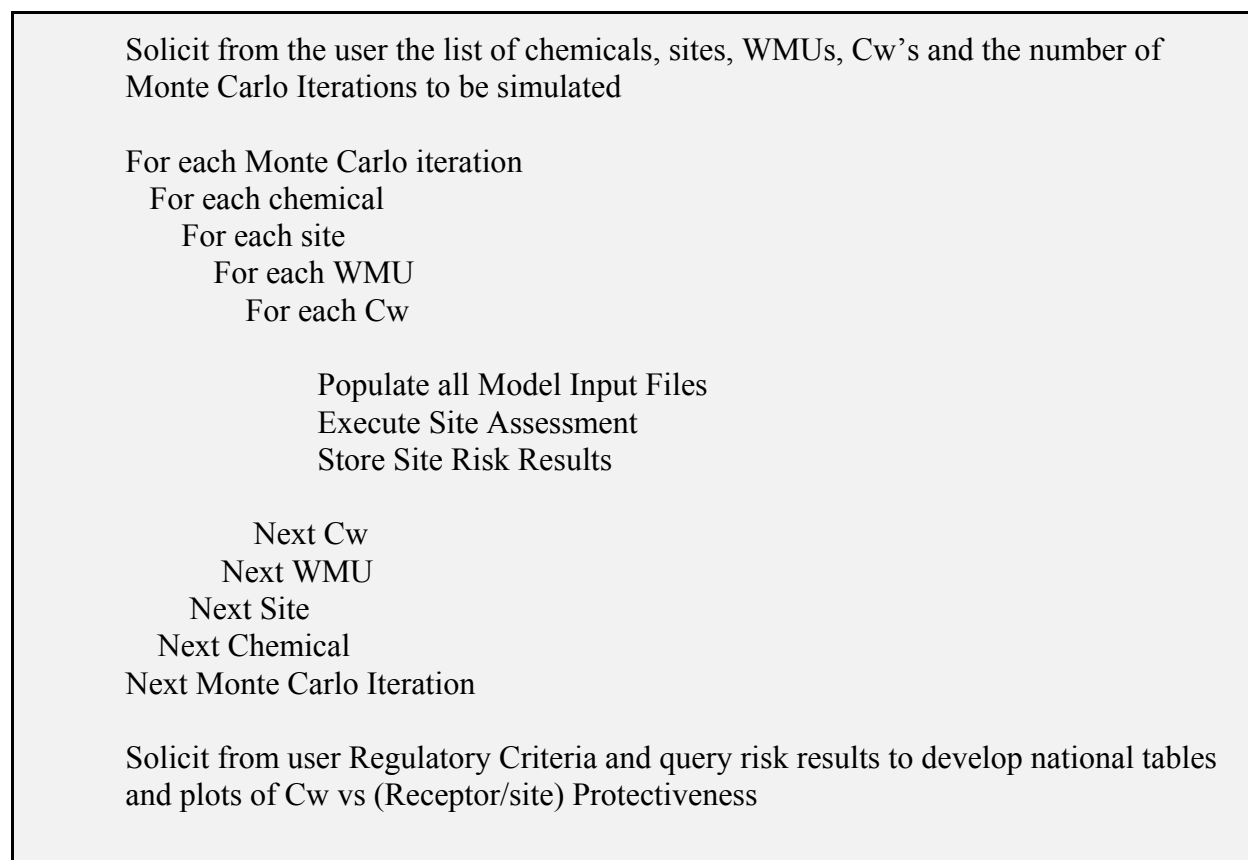


Figure 3.1 3MRA National Assessment High Level Algorithm

Figure 3.2 presents a graphical view of the 3MRA modeling system design. The components of the system shown in Figure 3.2 include four types : science modules, databases, system processors, and system data files. The roles and relationships among the components can be concluded from their form and organization in the graphic. However, the operational relationship among the components, that is, the programming standards and system utilities that establish and facilitate the data and execution management protocols for the system, are not shown in Figure 3.2, but are critical to appreciating the full design. The following brief description of the components and programming aspects of the system design presented in Figure 3.2 provides a big picture or framework view of the system that forms the basis for understanding progressively more detailed descriptions presented in subsequent sections. Sections 3.2.1 through 3.2.6 provide descriptions of the major features of the 3MRA modeling system.

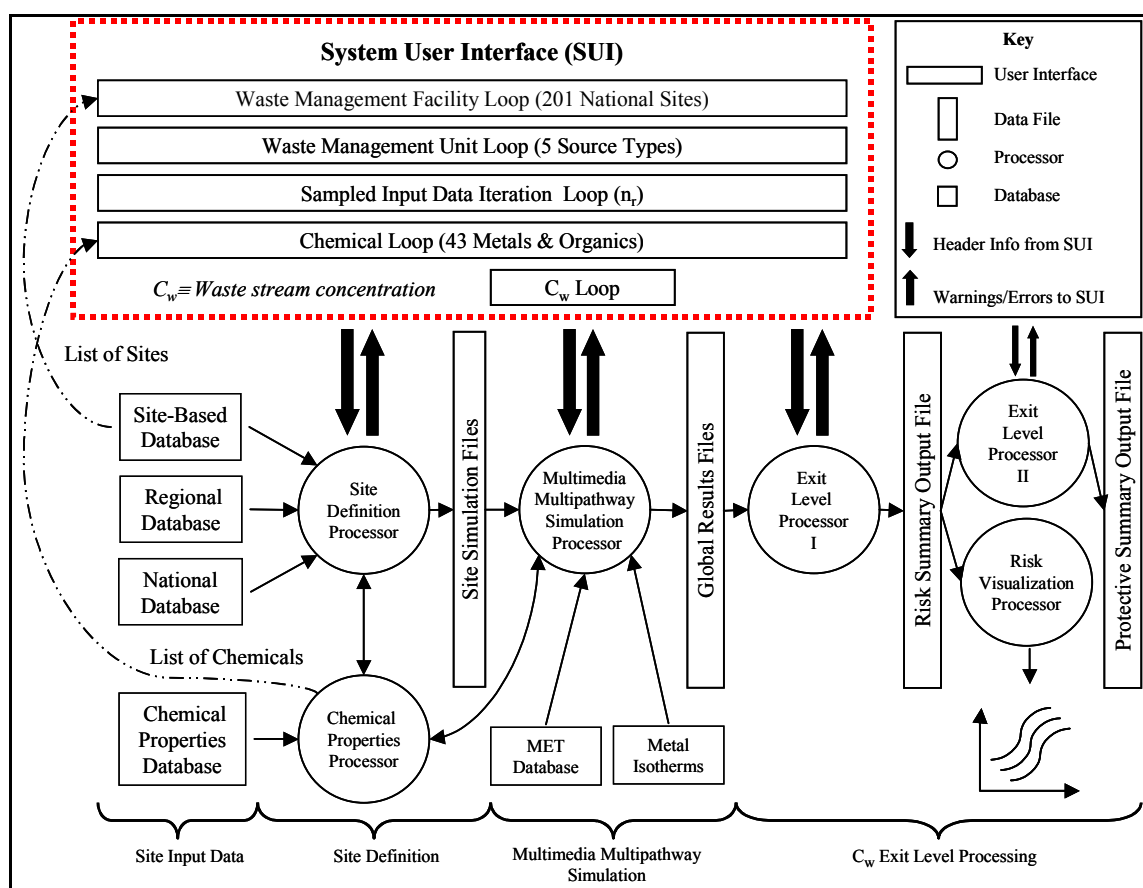


Figure 3.2 3MRA System Design

3.2.1 Science Modules

The extensive site scale modeling required for 3MRA was partitioned into logical units based on “real world” objects (representing, essentially, well bounded environmental media and processes such as a “watershed” and “aquatic foodweb”). The resulting set of science modules and their logical connectivity (i.e., data dependency relationships) are illustrated in Figure 3.3. The individual science modules include five source release modules (land application unit,

landfill, surface impoundment, aerated tank, and wastepile), five media-specific fate and transport modules (watershed, atmospheric, vadose zone, aquifer, and surface water), a farm foodchain module, two foodweb modules (terrestrial and aquatic), and two exposure and two risk modules (human and ecological).

In the system diagram they are represented by the circle in the center of the diagram labeled Multi-media, multi-pathway Simulation Processor (MMSP). This collection of science modules represents a modeling system or domain that is, itself, contained in the larger 3MRA modeling system. The coordinated execution of the modules is managed by the MMSP.

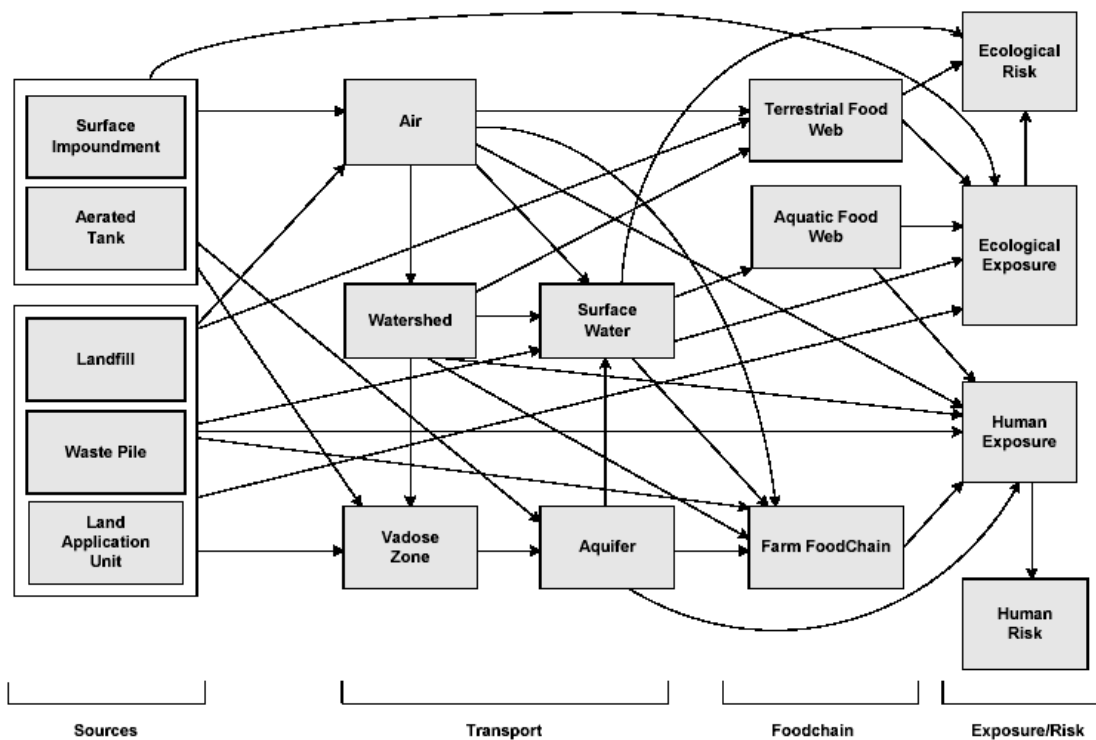


Figure 3.3 3MRA Science Modules and Related Connectivity

3.2.2 System Databases

The following system databases are included in the 3MRA modeling system.

Site-based Database: Contains all data associated with specific 3MRA sites. There are 201 unique site locations, each containing one or more waste management units. There are a total of 419 combinations of site and WMU.

Regional Database: Contains data associated with variables that are characterized on a regional geographic basis. All data contained in the regional database is in the form of a statistical distribution to facilitate sampling and assignment to specific sites.

National Database: Contains data associated with variables that are characterized on a national geographic basis. All data contained in the national database is in the form of statistical distribution to facilitate sampling and assignment to specific sites.

Chemical Properties Database: A series of data files that contain all chemical-specific data (e.g., anaerobic biodegradation rate constants, health effects data).

Meteorological Database: A series of data files that contain meteorological data for weather stations across the U.S. The MET data is provided in various temporal formats including hourly, daily, monthly, annual, and long term average.

Metal Isotherm Database: Database used by groundwater modules (vadose and aquifer) only. Contains media partitioning data for metals.

3.2.3 System Processors

The system processors collectively manage the execution of the 3MRA modeling system. Processors interact with the user, develop science module input data files, manage the execution of the of individual system components, and process modeling outputs to form national risk summaries. The 3MRA Processors are as follows :

System User Interface (SUI) : this processor represents the user access point to the technology. Via the SUI the user selects which combinations of sites, waste management units, chemicals, constituent concentrations in waste streams to be simulated, and the number of Monte Carlo simulations to be executed per site. The SUI also provides the user with the ability to configure the computer directory structure where individual components of the system are stored. Finally, the SUI manages the overall execution of the user defined national assessment.

Site Definition Processor (SDP) : this processor performs all data retrieval from the site, regional, national, and chemical databases and organizes it into a series of “site simulation files” that contain the input data for each of the seventeen science models.

Multi-media Simulation Processor (MMSP) : this processor manages the invocation, execution, and error handling associated with the seventeen individual science models that simulate source release, multimedia fate and transport, foodweb dynamics, and human/ecological exposure and risk.

Chemical Properties Processor (CPP) : this processor accesses the chemical properties database and either transfers or calculates all requested data. The CPP represents a single location within the modeling system where chemical data is made available.

Exit Level Processor I (ELP I) : this processor assimilates the individual site risk results and builds a risk summary database containing data used to assess national protection criteria.

Exit Level Processor II (ELP II) : this processor reads the ELP I derived risk summary database and generates, based on regulatory criteria, specific national exemption levels.

Risk Visualization Processor (RVP) : accessed through the ELP II (and thus effectively a sub-component of the ELP II) this processor presents national risk summary results in graphical form.

3.2.4 System Data Files

System data files are those that are created during execution of the 3MRA modeling system. The following system data files are included in design.

Site Simulation Files (SSFs): Files containing general simulation information and input data for individual science modules. The SSFs are produced by the Site Definition Processor based on general simulation instructions from the SUI and the SDPs access to the set of 3MRA system databases.

Global Results Files (GRFs): Files generated by individual science modules containing module simulation results. A single GRF is produced by each science module but may be consumed by multiple science modules that execute after the producing module (e.g., the source GRF contains inputs, and is then consumed by the individual media fate and transport modules).

Risk Summary Output File (RSOF) : Files generated by the ELP I Processor and containing site-based risk data in a condensed format for use in developing national protectiveness summaries.

Protective Summary Output File (PSOF) : Files generated by the ELP II Processor and containing tables of national regulatory limits per regulatory scenario (i.e., combination of protectiveness criteria and decision factors, e.g., combination of waste management units, human and ecological receptors of concern, exposure pathways, etc.).

Miscellaneous Data Files: Within the 3MRA modeling system science modules, particularly legacy models, may require input data files in the original model format and produce output data files not used by the 3MRA system. These files are read and written by module-specific pre- and post-processors that function as translation routines facilitating communication of data from the 3MRA system to/from legacy modules.

3.2.5 Programming Standards and System Utilities

Within the 3MRA modeling system there are specific design features that represent “standard protocols” that must be included as part of any components implementation. These standards ensure the consistent and accurate transfer of information throughout the system. In addition, 3MRA includes utilities to facilitate specific types of data preparations and transfers. The following standards and utilities are included in the 3MRA technology design.

Data representation standard : With the combination of the sheer number of variables included in the modeling system and the need to share the data among numerous systems components the 3MRA design team developed a standard means for defining and referencing data. This is the most fundamental aspect of the 3MRA modeling technology system. In 3MRA, data is assigned to a specific data file that is itself associated with a particular science module or system processor. Further, each variable is defined with the following attributes : Name, Dimensions, Data Type, Min, Max, Units, Description, Dimensional Indices. These metadata for the modeling variables are contained within a DICTIONARY file. A dictionary file is assigned to each modeling file and used by the IO dll (see below) to retrieve and assign data to files. During execution, each software component in the system must repeat the attributes of a variable whenever it attempts to either read or write a value for the variable.

Input/Output Dynamic Linked Library (IO dll) : this utility contains a library of routines that perform all the functions needed to open/close files, read/write data from databases and inter-model files, and perform QA checks on each data transfer. This processor acts as an Application Programming Interface (API) and is designed to be functional in multiple computer languages (i.e., C, C++, FORTRAN, Visual Basic, and Java). All system components utilize this common API to effect data transfers.

Monte Carlo Dynamic Linked Library (MC dll) : this utility contains a library of routines to perform all the functions needed to randomly sample data values, including correlated data, from defined statistical distributions.

3.2.6 Integrated Functionality of 3MRA Modeling System

The 3MRA national assessment methodology that applies the science modules and related data is reflected in Figure 3.2 in the box labeled System User Interface (SUI) and the Exit Level Processors I and II. Within the SUI the nested loops that reflect the combinations of simulation factors that are needed to conduct a national assessment are shown. The SUI acts as a dispatcher, first interacting with the user to determine which combination of site assessment factors should be executed and then methodically invoking the SDP, MMSP, and ELP I to populate the SSFs with data from the 3MRA databases, execute the individual site simulations, and store the necessary risk summary data, respectively.

As described earlier the 3MRA methodology includes a two-stage Monte Carlo simulation capability. The first stage is represented by the site loop, that is, a single execution of all the sites. The second stage is reflected in the SUI loop entitled “Sampled Input Data Iteration”. This stage of Monte Carlo simulation executes the first stage repetitively, i.e., multiple executions of the set of sites.

When all site simulations are complete the RSOF is populated with all risk summary data needed to generate national level expressions of risk protectiveness. The ELP II conducts the national roll up. The ELP II invokes the RVP to request from the decision analyst the regulatory scenarios of interest. The RVP displays plots of national scale probability of protectiveness and allows the user to view calculated regulatory limits that result from the specific regulatory criteria. The ELP II generates tables containing the national regulatory limits.

3.3 Component Design

The previous discussion provided an overview of how the 3MRA technology requirements were transcribed into an integrated software system design. While attention was paid to the individual components of the system the focus was a description of how the components inter-relate in order to automate the 3MRA national assessment methodology. The purpose of this section is to provide additional detail concerning the components of the 3MRA software system.

Included in this discussion are the following design elements and features :

- Data Representation Standard [Section 3.3.1]
- Data Exchange Utility (IOdll) [Section 3.3.2]
- Monte Carlo Sampling Utility (MCdll) [Section 3.3.3]
- Chemical Properties Processor (CPP) [Section 3.3.4]
- 3MRA Databases [Section 3.3.5]
- System User Interface (SUI) [Section 3.3.6]
- Site Definition Processor (SDP) [Section 3.3.7]
- Multimedia, Multipathway Simulation Processor (MMSP) [Section 3.3.8]
- Exit Level I Processor (ELP I) [Section 3.3.9]
- Exit Level II Processor (ELP II) [Section 3.3.10]

3.3.1 Data Representation Standard for the 3MRA Modeling System

To perform a comprehensive site-scale human and ecological risk assessment requires a significant amount of environmental data. The data characterizes the inter-related physical features of the site (e.g., watersheds, surface waters, aquifers, ecological habitats, population distributions, land uses, etc.) along with the detailed data describing the physical, chemical, and biological processes effecting the fate, transport, uptake, exposure, and risk associated with contaminant releases to the environment. Data required for any given site (of the 201 included in the 3MRA database) amounts to several hundred variables. These data are extracted from the central databases (i.e., Site, Regional, National) by the Site Definition Processor (SDP) which, in turn, organizes specific input files for each of the seventeen science modules contained in the 3MRA modeling system. The science modules themselves produce output information (e.g., concentration time series) that is consumed by yet other modules. The point here is that within a 3MRA-based national risk assessment there are terabytes of data produced and consumed. Obviously, not all the data can be archived, yet it is essential that each and every data transfer be correct. To this end, the 3MRA technology design includes a formal mechanism for ensuring the quality of data, its representation, and its transfer among components of the system.

All data that is transferred within the 3MRA modeling system, whether it be from the central databases through the SDP to the SSFs or from one science module to another via GRFs, is formally identified with a series of attributes. The attributes reflect the metadata of the data and include the following : Variable Name (Code), Dimensions, DataType, Min, Max, Units, Description, Dim1, Dim2, Dim3. The metadata that describes the attributes of each individual data item is stored in system files referred to as DICTionary files. A dictionary file is assigned to each modeling file. Figure 3.4 illustrates the system context of DICTionary files within the 3MRA software system. One DIC file exists for each data file included in the system. While

each data file contains the numerical value for the variable, each associated DIC file contains the meta data (the data attributes).

To illustrate this concept further Table 3.1 contains the numerical data associated with a Site Simulation File for the Watershed Module. Note that in addition to the numerical value per variable there are additional entries. These entries refer to the variable metadata. The definition of the meta data is contained in the associated DIC file shown in Table 3.2. While the metadata concept and dictionary files provide the information to ensure data quality within the 3MRA modeling system it must be implemented in a formal manner by all software (i.e., system processors and science modules). This is achieved in 3MRA with an Input/Output Dynamic

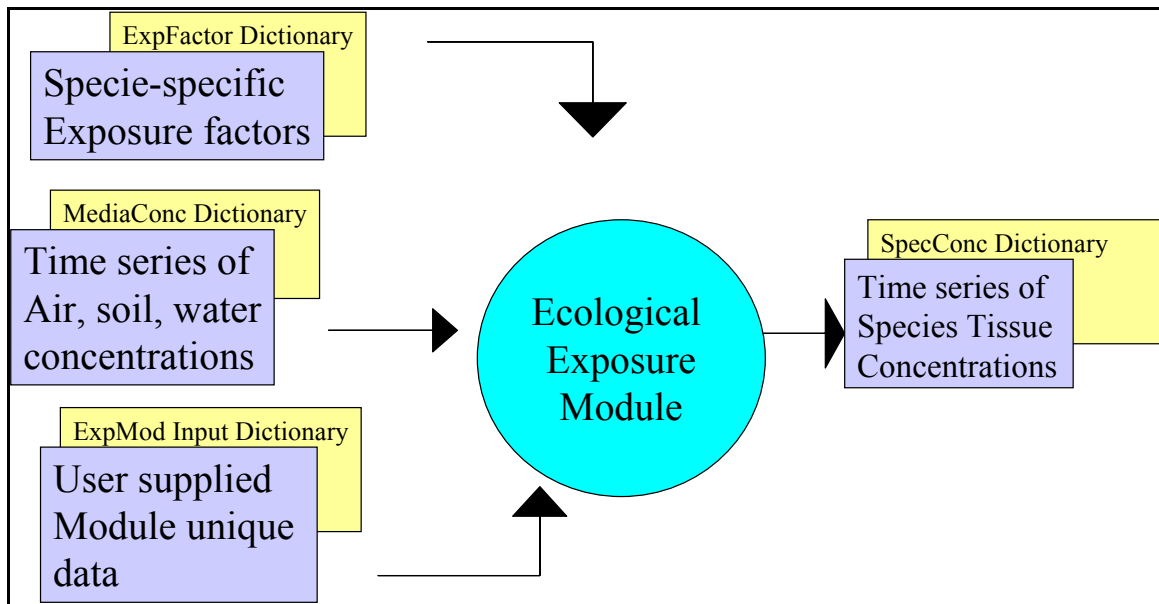


Figure 3.4 3MRADictionary Files

```

1,
"wsWPMaineHg.ssf","data group",
23,
"a_BF",0,"FLOAT",0,"m/d",
1.08e-005,
"b_BF",0,"FLOAT",0,"unitless",
1.16,
"bcm",0,"FLOAT",0,"unitless",
1,
"C",1,"FLOAT",0,"unitless",
5,0.00510101,0.005045328,0.00961849,0.009241012,0.021134361,
"CN",1,"FLOAT",0,"unitless",
5,72.8989899,73.08158996,74.17942708,73.78739458,75.25770925,
"ConVs",0,"FLOAT",0,"m/d",
0.287852011,
"deltDiv",0,"INTEGER",0,"unitless",
1,
"DRZ",1,"FLOAT",0,"cm",
5,197.979798,199.7008368,191.6338542,193.2232579,176.1674009,
"Infild",0,"FLOAT",0,"m/d",
0,
"K",1,"FLOAT",0,"kg/m2",
5,0.18,0.18,0.18,0.18,0.18,
"Ksat",1,"FLOAT",0,"cm/h",
5,2.123995151,10.85980699,1.664272109,1.043309383,0.1275850911,
"P",1,"FLOAT",0,"unitless",
5,1,1,0.972005208,0.973146915,0.895374449,
"RunID",0,"STRING",0,"",
"Version25",
"SMb",1,"FLOAT",0,"unitless",
5,4.9,4.9,4.9,4.9,4.9,
"SMFC",2,"FLOAT",0,"volume %",
5,
4,22.5,23.2,22.9,21.3,
4,22.5,23.2,22.9,21.3,
4,22.5,23.2,22.9,21.3,
4,22.5,23.2,22.9,21.3,
4,22.5,23.2,22.9,21.3,
"SMWP",2,"FLOAT",0,"volume %",
5,
4,10.4,12.1,11.9,11.5,
4,10.4,12.1,11.9,11.5,
4,10.4,12.1,11.9,11.5,
4,10.4,12.1,11.9,11.5,
4,10.4,12.1,11.9,11.5,
"Theta",1,"FLOAT",0,"degrees",
5,2.919734303,2.919734303,3.662160152,2.176326011,2.46235273,
"thetawZ1d",0,"FLOAT",0,"volume fraction",
0,
"WCS",1,"FLOAT",0,"volume fraction",
5,0.41,0.41,0.41,0.41,0.41,
"X",1,"FLOAT",0,"m",
5,39.26400663,46.74481561,37.60883794,51.55062411,62.55905807,
"zava",0,"FLOAT",0,"m",
0,
"zavb",0,"FLOAT",0,"m",
0.05,
"zZ1sa",0,"FLOAT",0,"m",
0.05,

```

Table 3.1 Example 3MRA Data File : Watershed Site Simulation File (ws.ssf)

Linked Library (IODll), as described in the next section.


```

24,watershed,,,,,,,,,
Code,Dimensions,DataType,Min,Max,Units,Description,Dim1,Dim2,Dim3
a_BF,0,float,0,1000,m/d,regression coefficient a for baseflow model,,,
b_BF,0,float,0,10,unitless,regression coefficient b for baseflow model,,,
bcm,0,float,0,1,unitless,boundary condition multiplier (lower boundary),,,
C,1,float,0,1,unitless,USLE cover factor,NumWSSub,,
CN,1,float,0,100,unitless,SCS curve number,NumWSSub,,
ConVs,0,float,0,10,m/d,settling velocity (suspended solids),,,
deltDiv,0,integer,1,10,unitless,time step divider (for debugging),,,
DRZ,1,float,0,1000,cm,depth (root zone),NumWSSub,,
Infil,0,float,0,100,m/d,input infiltration rate (for debugging),,,
K,1,float,0,1,kg/m2,USLE erodibility factor,NumWSSub,,
Ksat,1,float,0,0.0000001,1000000,cm/h,saturated hydraulic conductivity (soil),NumWSSub,,
P,1,float,0,1,unitless,USLE erosion control factor (watershed j),NumWSSub,,
RunID,0,string,,,,run identification label (optional),,,
SMb,1,float,0,12,unitless,soil moisture coefficient b,NumWSSub,,
SMFC,2,float,0,100,volume %,soil moisture field capacity,NumWSSub,nlayer,
SMWP,2,float,0,100,volume %,soil moisture wilting point,NumWSSub,nlayer,
Theta,1,float,0,75,degrees,slope (watershed),NumWSSub,,
thetawZ1d,0,float,0,1,volume fraction,input volumetric water content in till zone (for debugging),,
WCS,1,float,0,1,volume fraction,saturated water content (total porosity),NumWSSub,,
X,1,float,0,50000,m,flow length (watershed),NumWSSub,,
zava,0,float,0,10,m,averaging depth upper (depth averaged soil concentration),,,
zavb,0,float,0,0.01,100,m,averaging depth lower (depth averaged soil concentration),,,
zZ1sa,0,float,0,0.01,1,m,depth (modeled soil column),,,

```

Table 3.2 Example 3MRA DIC File for Watershed Site Simulation File (ws.dic)

3.3.2 Input/Output Dynamic Linked Library (IODll)

The purpose of the IODll is to standardize and facilitate the exchange of data among system components of the 3MRA technology. The IODll is a library of utilities that contains all the functions needed to open/close files, read/write data from databases and inter-module files (i.e., SSFs/GRFs), and perform QA checks on each data transfer. The IODll acts as an Application Programming Interface (API) and is designed to function with multiple computer languages (i.e., C, C++, FORTRAN, Visual Basic, and Java). All system components utilize this common API to effect data transfers.

The design of the 3MRA IODll encompasses several subroutines and functions, including those for initialization, input, output, and finalization. In summary, the subroutines and functions include the following:

FUNCTION	DESCRIPTION
Subroutine OpenGroups	This subroutine is expected to be the first call in a program and to first retrieve the call arguments and open the warning and error files. If the warning and error files are opened successfully, all appropriate data groups are opened with the correct read/write mode.
Subroutine CloseGroups	This subroutine is expected to be the last call in a program and to close all data group, warning, and error files. It then destroys the error file, signaling to the SUI that no error occurred in the component.
Function ReadInt	This function returns the integer value for the given data group, variable name, and set of indexes.
Function ReadReal	This function returns the real value for the given data group, variable name, and set of indexes.
Function ReadLogical	This function returns the logical value for the given data group, variable name, and set of indexes.
Subroutine ReadString	This subroutine returns for the variable <i>String</i> , the string value for the given data group, variable name, and set of indexes.
Subroutine NumArgs	This subroutine returns the number of call arguments handed to a module.
Function GetArgInt	This function returns the integer value for the given call-argument index.
Subroutine GetArgString	This subroutine returns the string value for the call-argument index.
Subroutine WriteInt	This subroutine stores the given integer value in the given data group, variable name, and set of indexes.
Subroutine WriteReal	This subroutine stores the given real value in the given data group, variable name, and set of indexes.

Subroutine WriteLog	This subroutine stores the given logical value in the given data group, variable name, and set of indexes.
Subroutine WriteString	This subroutine stores a string of up to 80 character values in the given data group, variable name, and set of indexes.
Subroutine Error	This subroutine will add the string value passed by the calling program to the error file and then terminate the calling program.
Subroutine Warning	This subroutine will add the string value passed by the calling program to the warning file and then return control to the calling program.

In addition, the 3MRA IOdll performs Quality Assurance checks on all data transfers. To accomplish this it is required that all software within the 3MRA modeling system read and write data using the IOdll. This requires that the read and write statements include the attributes of the data item (including the name of the file within which the variable/value is to be located). The IOdll checks to ensure that the attributes stated by the reading/writing code are consistent with the attributes contained in the DIC file containing the variable of interest. For example, if a science module coded in FORTRAN contained the following line of code:

```
MyInts(i,j,k)=ReadInt3("Source_SSF," "XYZ," "cm/s,"i,j,k)
```

the IOdll will execute the following QA tests :

- 1) Does the science module data group "Source_SSF" exist? If not, raise an error.
- 2) Does the variable "XYZ" exist in "Source_SSF"? If not, raise an error.
- 3) Are any of the indexes negative? If so, raise an error.
- 4) Do the specified units for "XYZ" in "Source_SSF" match the units passed by the calling program? If not, raise an error.
- 5) Does the specified dimensionality of "XYZ" match the calling program's assumptions of dimensionality? If not, raise an error.
- 6) Is any one of the indexes larger than the maximum indexes stored in the file? If so, raise a warning and return a 0.
- 7) Is the value stored in the data file outside the specified bounds for that variable? If so, raise an error.
- 8) Does the specified type of the variable match the assumed type from the calling program? If not, raise an error.

3.3.3 Monte Carlo Sampling Dynamic Linked Library (MCdll)

One of the requirements for the 3MRA modeling system is that all variables contained in the site, regional, and national databases be optionally characterized as stochastic. The intent of this requirement is to facilitate Monte Carlo-based simulations where individual variables that are either naturally variable in nature or their value is uncertain can be assigned values from a statistical distribution.

To satisfy these requirements and to provide a single source of such statistical sampling within the modeling system the 3MRA technology design includes a Monte Carlo dynamic linked library (MCdll) that contains a core set of Monte Carlo functions and subroutines.

The 3MRA MCdll includes the following statistical distribution types; Normal, LogNormal, JohnsonSB, Transformed LogNormal, Exponential, Triangular, Uniform, Integer Uniform, SB, SU, Gamma, Weibull, and Empirical. The MCdll allows correlation among the variables.

A key feature of the MCdll implementation is that the random number seed is set as an input parameter rather than, for example, being set by an internal routine. This standardization of the random number sequence allows for explicit reproducibility of results. This is critical both in the software development phase as well as in the context of regulatory applications.

The 3MRA MCdll is comprised of the following subroutines:

FUNCTION	DESCRIPTION
Subroutine StatNumDist	This subroutine sets the number of distributions that will have values sampled from them.
Subroutine StatNumCor	This subroutine sets the number of correlations between the given distributions that will have values sampled from them.
Subroutine StatDebugOn	This subroutine will turn on debug messages in the MCdll.
Subroutine StatSeed	This subroutine sets the seed to be used by the MCdll. This allows for a reproducible set of samples from the given set of distributions.
Subroutine StatClear	This subroutine deallocates any memory resources used by the MCdll.
Subroutine StatCor	This subroutine sets a correlation between two distributions.
Subroutine StatSample	This subroutine performs the sampling from the given set of distributions.
Distribution Definition Functions	In general, the Distribution Definition Functions provide the MCdll with the parameters for a specific distribution type. For example, the Normal() function sets the mean, standard deviation, minimum, and maximum for a normal distribution.

While the MCdll is accessible by any 3MRA processor or science module it is the case that the Site Definition Processor (SDP) executes all statistical sampling. This centralization of the Monte Carlo sampling is designed for efficiency and quality assurance.

3.3.4 Chemical Properties Processor (CPP)

The Chemical Properties Processor (CPP) represents the single source of chemical-specific data in the 3MRA modeling system. The CPP represents a library of subroutines and functions that receive requests for specific chemical property data, accesses the relevant chemical data file(s), performs any required computations, and returns a value for the requested property.

Within the 3MRA design the CPP receives requests for chemical property data either from the Site Definition Processor (SDP) or directly from the science modules. The protocol followed is that the SDP, which is responsible for populating all module input files (i.e., Site Simulation Files - SSFs), requests chemical data from the CPP, which, in turn, accesses a series of specific data files, each containing a group of chemical data, and either transfers directly or derives the requested chemical property value. In the event that a science module simulates environmental conditions that affect the value of a chemical property (e.g., temperature and pH effects on physical properties of organic compounds) the science module can access the CPP and 1) provide the environmental conditions, and 2) request, in return, appropriate condition-specific chemical property values.

The 3MRA modeling system contains the following series of chemical property data files:

- Organic Chemical Property (OCP)
- Metal/Inorganic Chemical Property (MICP)
- Transformation Products (TP)
 - Catalyzation (CAT)
 - Aerobic Biodegradation (AerBio)
 - Activated Biodegradation (ActBio)
 - Anaerobic Biodegradation (AnaBio)
 - Anaerobic Reduction Biodegradation (AnaRedBio)
 - SO₄ Reduction Biodegradation (SO4Bio)
 - Methanogenic Biodegradation (MethBio)
- Human Health Benchmarks (HHB)
- Ecological Benchmarks (EB)
- Ecological Bioaccumulation Factors (EBF)
- Aquatic Bioaccumulation Factors (ABF)
- Chemical Ecological Flag

These files are designed and maintained as comma delimited ASCII data files. As such access and retrieval of data is efficient and the files are easily assimilated into standard spreadsheet software for review and modification.

The CPP is designed as a dynamic link library (DLL) to facilitate consistent communication between components. The CPP contains a series of subroutines and functions that retrieve chemical data from the files and perform any necessary calculations. For example, the following set of subroutines is included for accessing the Organic Chemical Property (OCP) data:

CPP Function for OCP	Description of Function
Function ChemADiff	This function computes the air diffusion coefficient for organic chemicals, in cm ² /s.
Function ChemVol	This function computes the volume for organic chemicals, in mL.
Function ChemDen	This function computes the density for organic chemicals, in g/mL.
Function ChemWDiff	This function computes the water diffusion coefficient for organic chemicals, in cm ² /s.
Function ChemVP	This function computes the vapor pressure for organic chemicals, in torr.
Function ChemSol	This function computes the solubility limit for organic chemicals, in mg/L.
Function ChemHLC	This function computes the Henry's Law Constant for organic chemicals in (atm m ³ / mol).
Function ChemKow	This function computes the Kow for organic chemicals (dimensionless).
Function ChemKoc	This function computes the Koc for organic chemicals in mL/g.
Function ChemHyd	This function computes the hydrolysis rate for organic chemicals in 1/day units.

There are two sets of subroutines included in the CPP that do not return specific chemical property data. The first set of subroutines initialize the CPP, that is, the initialization subroutines establish the computer directory location where the chemical data files can be found, the chemical for which properties are to be determined, and the environmental conditions relevant for computing the chemical property (i.e., pH, temperature, and environmental media). The second set of subroutines that do not return specific chemical property data inform the calling program about 1) the SMILES string for organic chemicals, 2) the number of valid chemicals for which the CPP has properties (if a chemical is missing part of its required data, it will not be included in this count), and 3) to create a list of the available chemicals (and their associated index, name, and CASID) available in the chemical property file being read by the CPP.

Requests for all other chemical properties are processed with individual subroutines or function calls specific to the property of interest. In the case when chemical transformation rates are involved it may also be the case that the transformation reaction results in the formation of chemical products. For all transformation related chemical properties (e.g., biodegradation rate constant) the calling program can also request information about the number and name of chemical products and the yield coefficients associated with the transformation reaction.

3.3.5 3MRA Databases and Data Files

Within the 3MRA modeling system there are three main categories of data; input, intermediate, and output. Input data includes all data needed to simulate a comprehensive multimedia risk assessment at each of 201 sites. Intermediate data includes information produced for or by any of the science modules within the modeling system. The intermediate files produced by the science modules contain times series predictions of variables associated with individual science modules (e.g., concentration time series). These intermediate files report data on an annual basis (some modules internally process time steps shorter than one year but report results only on an annual basis). 3MRA output files contain protection data, that is, the end result of all the site-based simulations are data matrices that contain information necessary to determine percentages of national population (human and ecological) and/or waste management unit sites that are protected from risk/hazard quotient values greater than a policy prescribed threshold.

The following three sections provide summary descriptions of the three categories of data.

3.3.5.1 3MRA Input Data

The 3MRA input data includes site, waste management unit, chemical, and meteorological data. The site data includes both site layout and site environmental setting information. The site layout data reflects all the physical features of the site and their interconnectivity. Features included in the site layout data for 3MRA include :

- Waste Management Unit (WMU)
- Watershed(s)
- Surface Water Network(s)
- Aquifer(s)
- Ecological Habitat(s)
- Ecological Home Ranges per Specie
- Human Population Distribution

Site environmental setting data includes the following data groups :

- Atmosphere
- Surface water
- Watershed soils/cover
- Vadose zone
- Aquifer
- Terrestrial and aquatic foodwebs
- Farm foodchain
- Waste Management Unit characteristics

As described earlier the site environmental data is assigned via a hierarchical protocol for populating the series of Site Simulation Files (SSFs) that form the input for the individual science modules. The protocol calls for a series of three data tables, each reflecting a higher spatial representation of the data. The site data table contains data that has been collected for a specific site. If data for a site does not exist the 3MRA modeling system (i.e., the SDP) scans

the regional data set. If the SDP finds the variable in the regional data set a value is extracted (may be sampled using the Monte Carlo DLL) and placed in the appropriate SSF. Finally, if the variable is not located in either the site or regional data set the SDP scans the national data file for appropriate information from which to derive a site value to be used during simulation.

Also included in the 3MRA input data are chemical and meteorological data. Chemical properties are included in a series of files that are organized by the type of property. The categories of chemical properties included in 3MRA are :

- Physical Property
- Chemical and biological transformation rates (with products of transformation)
- Biouptake and bioaccumulation factors
- Metal Isotherms
- Human and ecological health benchmark

The chemical data is stored in a series of comma delimited ASCII files that facilitate their access by system processors and models and their overall maintenance. The data is read from the data files by the CPP (primarily upon request of the SDP) using the same IODll used by all other processors and models in the modeling system. This provides for, as described earlier, a high degree of quality assurance in the use of the data.

The last category of input data contained in the 3MRA modeling system is the meteorological data. Because the science modules contained in 3MRA may simulate processes at time steps less than the reporting time step (i.e., annual) the MET data must be available for hourly, daily, and monthly time frames as well as annual and long term average. Most meteorological data were extracted from Solar and Meteorological Surface Observation Network (SAMSON) hourly data files and converted as necessary to daily time series, monthly time series, annual time series, and long-term averages.

Table 5.3 lists the specific meteorological data needs of the 3MRA modeling system and the time frames needed for each of the data items.

Table 3.3 3MRA MET Data

MET Variable	Hour	Day	Month	Annual	Long Term
Surface roughness length	✓				
Minimum Monin-Obukhov length	✓				
Friction velocity	✓				
Precipitation code	✓				
Stability category	✓				
Cloud cover		✓	✓		✓
Temperature	✓	✓	✓	✓	✓
Wind direction	✓				

Windspeed	✓	✓	✓	✓	✓
Precipitation	✓	✓	✓	✓	✓
Evaporation		✓	✓	✓	✓
Windspeed at pile height		✓			
Number hours wind > 5.4 m/s at pile height		✓			
% time wind > 5.4 m/s at pile height				✓	
Thornthwaite precipitation-evaporation index (PE)				✓	
Days with precipitation > 0.01 in				✓	✓
Fastest mile of wind				✓	✓
USLE rainfall erosivity factor		✓			✓
Maximum/minimum temperature			✓		
Temperature of soil column					✓
Mixing height	✓				

Each site included in the 3MRA database is associated with one MET station set of data. This association is established principally as a function of proximity between the site and the station.

Finally, the meteorological data files are not designed for use within the 3MRA IODll construct, nor are they processed by the SDP with results incorporated into the Site Simulations Files. Rather, the MET files are contained in a series of standard data files for direct access by the science modules when needed. The primary reasons for this implementation strategy are simply resources and schedule.

3.3.5.2 3MRA Intermediate Data Files

There are two primary types of intermediate files contained in the 3MRA modeling system; Site Simulation Files (SSFs) that contain input data for the science modules and “header” information that describes runtime parameters, and Global Output Files (GRFs) that contain the results of individual science module simulations. The software design aspects of these files is described in Sections 3.3.1 and 3.3.2. Presented here is a brief description of the different types of SSF and GRF files based on their general content.

There are four types of SSF file within the 3MRA modeling system; Header SSF (hd.ssf), Site Layout SSF (sl.ssf), Chemical Data SSF (cp*.ssf), and Science Module SSF (*.ssf). The hd.ssf contains information associated with the overall simulation and includes data that

specifies the hard drive location on the host computer where all relevant files (data, modules, processors, etc.) reside. The sl.ssf contains data that describes the physical features of the site (i.e., area of interest surrounding a waste management unit) and their inter-connectivity, and as such, is accessed by several science modules. The chemical data required by the science modules is contained in a series of SSF files, one for each major media or science module. In all, there exist nine chemical SSF files in the 3MRA; source module (cpsr.ssf), watershed module (cpws.ssf), vadose zone module (cpvz.ssf), aquifer module (cpaq.ssf), farm food chain (cpff.ssf), human exposure module (cphe.ssf), and three files associated with the surface water module (for lakes [cpLake.ssf], streams [cpstream.ssf], and wetlands [cpwetland.ssf]).

The science modules each require a single input SSF that contains the values of variables unique to that module. Thus, there is a *.ssf for each of the seventeen 3MRA science modules in the system. Similarly, there is a *.grf for each of the science modules that contains the module output data. These data files may be saved by the user upon request, however, it is the case that if conducting a full national assessment it would be impossible to save all of the individual intermediate SSF/GRF files. Thus, saving the SSF/GRF files is generally useful when either executing a single site simulation, and this, in turn, has been useful in the context of verifying the proper functionality of individual science modules.

3.3.5.3 3MRA Output Data

There are two data files that are permanently stored as a result of a 3MRA national assessment simulation. The Risk Summary Output File (RSOF) contains a consolidation of the human and ecological risks estimated by the two science modules. The RSOF is appended to for each site simulation, thus, as the human and ecological risk modules complete their simulations the results are assimilated and stored in condensed form for later regulatory analysis. The second output file generated by the 3MRA modeling system is the Protection Summary Output File (PSOF). The PSOF contains final regulatory limits derived from applying regulatory criteria to risk/hazard data stored in the RSOF.

3.3.6 The System User Interface (SUI)

The System User Interface (SUI) has three primary roles within the 3MRA modeling system. First, the SUI is responsible for interaction with the user for the purpose of establishing the details of the site-based risk assessment to be executed. The SUI also manages the overall execution of the assessment process, processing the nested loops of Monte Carlo iterations, chemicals, sites, waste management units, and constituent concentration levels in the wastestreams. Finally, the SUI acts as the single source of warning and error messages that occur during execution. All messages, whether they are initiated within a science module or a system processor, are directed toward the SUI for final processing to the user.

The SUI, and indeed this version of the 3MRA technology, facilitates only assessments that utilize the site data contained in the 3MRA databases. While it is possible to execute the 3MRA technology for a site outside the 3MRA list there is no user interface to facilitate the input of site data.

3.3.6.1 User Interaction Features

The SUI represents the user access point to the technology. The SUI is a Windows™ menu-driven interface that collects information from the user and controls the activities associated with the simulation. The three main screens associated with the SUI are 1) SYSTEM CONFIGURATION, 2) SYSTEM MANAGEMENT, and 3) SYSTEM STATUS. These user interface screens are the main method of interaction between the user and the 3MRA modeling system.

The SYSTEM CONFIGURATION SCREEN, Figure 3.5, allows the user to specify the location on the host computer of all databases, data files, system processor executables, and science module executables for a simulation. There are seven system configuration screens, one of which, shown in Figure 3.5, accepts user specifications of the directory location of the individual media and transport modules (e.g., the vadose zone module resides on Drive: D within the 3MRA directory and is named vadose.exe).

The SYSTEM MANAGEMENT SCREEN consists of SELECTIONS AND OPTIONS subscreens. The SELECTIONS subscreen, Figure 3.6, allows the user to select the sites, chemicals, source types, and waste levels for simulation. The OPTIONS subscreen, Figure 3.7, allows the user to determine the storage level of input/output files for the simulation. The Minimum storage level saves only the Global Results Files (GRFs) for the simulation, and the Maximum storage level saves all processor and module files for the simulation. The OPTIONS

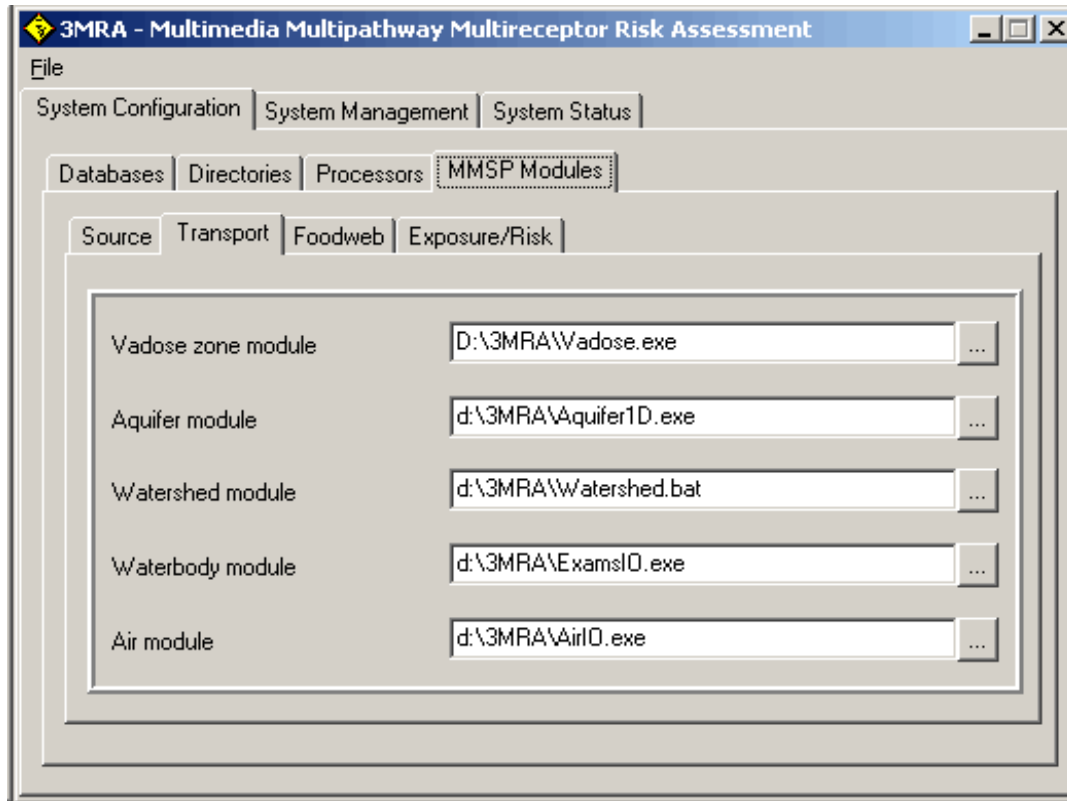


Figure 3.5 3MRA SUI System Configuration Screen

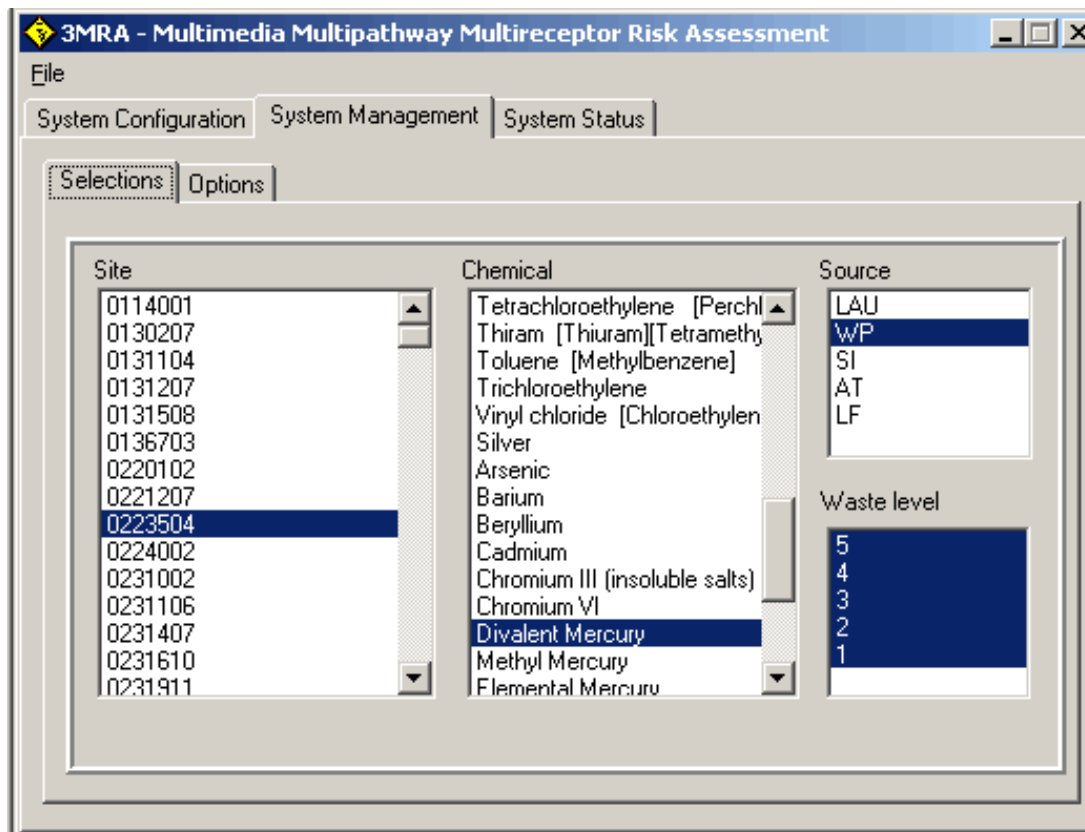


Figure 3.6 3MRA SUI Systems Management : Selections Screen

subscreen also allows the user to specify the number of Monte Carlo realizations for the simulation and the seed value used for the statistical sampling. This subscreen allows the user to specify the mode of operation for the simulation. These modes are: a) **Debug**, b) **Stop on Error** c) **Stop on Warning**, or d) any combination of these three modes. The **Debug** mode stops the simulation after every change in realization, chemical, source type, and waste level; the **Stop on Error** mode stops the simulation only if an error occurs in a processor or module; and the **Stop on Warning** mode stops the simulation only if a warning occurs in a processor or module. The user can select the **Debug**, **Stop on Error**, and **Stop on Warning** modes in different combinations to meet the needs of the simulation. The **Comment** box on this subscreen enables the user to enter descriptive information about the current simulation.

The SYSTEM STATUS SCREEN, Figure 3.8, informs the user of the status of the current simulation. Current realization, site, source type, chemical, and waste level are provided by this screen. Any error or warning message will display in the **Message** box on the screen and include which processor or module the message came from. This screen also has the **Start/Resume** button for the simulation. After stopping, the user can resume the simulation at anytime or use the **Reset** button to begin the simulation over (that is, put all the indexes back to the original settings and start the simulation from the beginning). This provides the user with full control over the simulation.

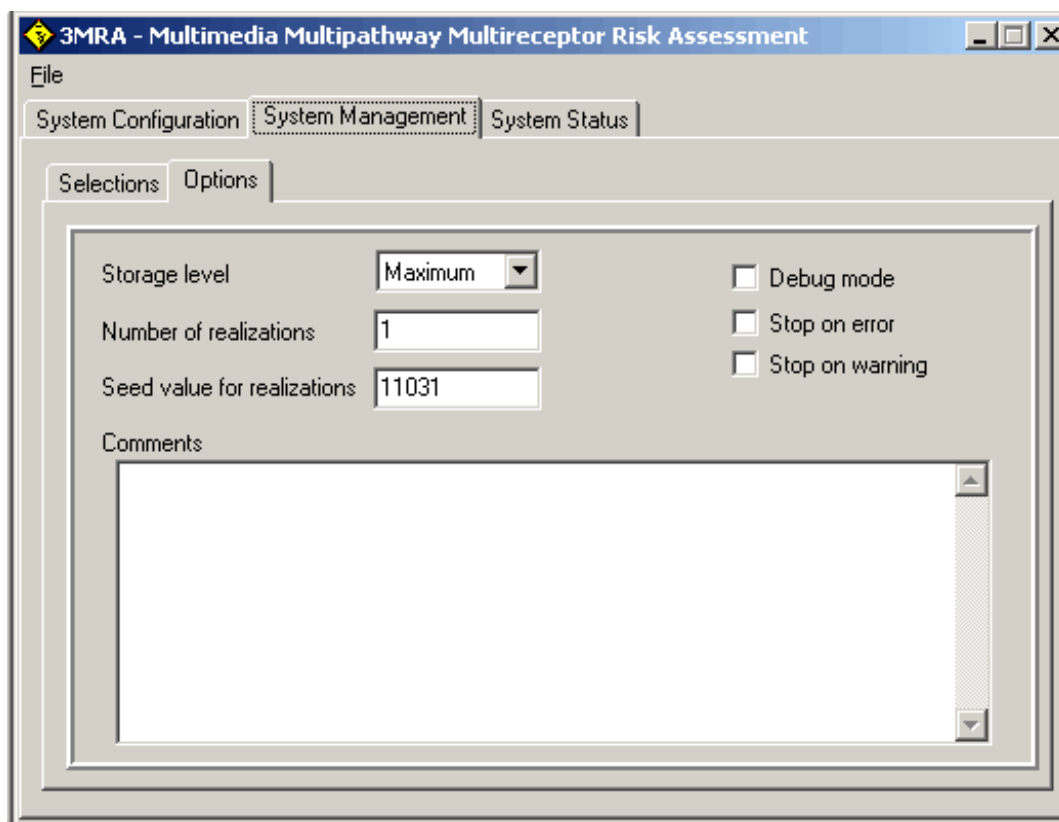


Figure 3.7 3MRA SUI System Management : Options Screen

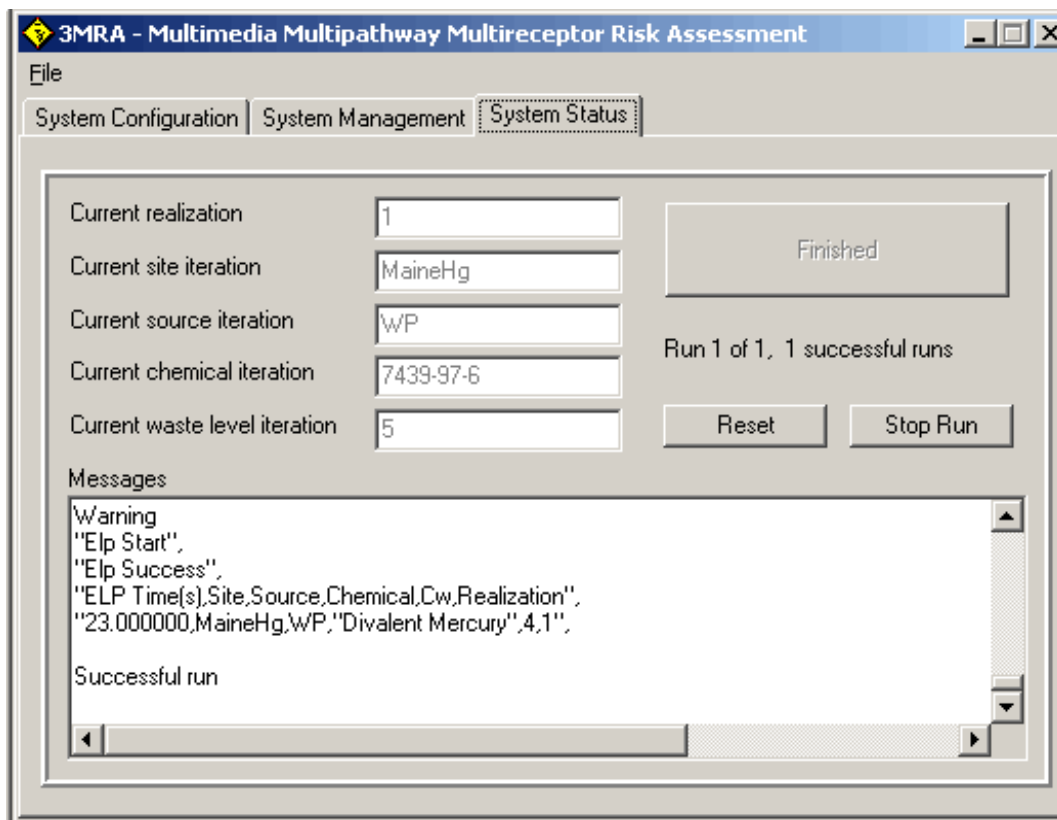


Figure 3.8 3MRA SUI System Status Screen

3.3.6.2 Execution Management Features

The SUI also manages the overall execution of the user specified assessment. As described above the user selects combinations of sites, chemicals, waste management units, constituent concentration levels in wastestreams, and the number of Monte Carlo realizations to execute. To implement the system, the SUI takes control over each of the system processors before the start of analysis and invokes processors in an ordered and logical manner.

Finally, the SUI receives and manages warning and error messages occurring in processors and modules. If the SUI receives a warning from a processor or module, the SUI displays the warning and continues (unless the **Stop on Warning** mode is selected, in which case the simulation stops) with the simulation in the SYSTEM STATUS SCREEN (see Figure 3.8). If an error is reported to the SUI, the SUI displays the error message and current state of the indexes and stops execution.

3.3.7 The Site Definition Processor (SDP)

The purpose of the SDP is to populate all Site Simulation Files (SSFs) needed to conduct individual site assessments required in the context of a 3MRA application. Site assessments are conducted for each combination of site, waste management unit, chemical, and chemical waste concentration requested by the user via the System User Interface. Thus, for example, if the user selects 30 sites, 4 chemicals, 2 waste management units, and all 5 waste concentration levels

there would be a total of 1200 individual site risk assessments executed during the single session initiated by the user. The SDP, under the control of the SUI, gathers data for each site risk assessment from the Site Variable Distribution Table, Regional Variable Distribution Table, National Variable Distribution Table, and Chemical Properties Database and transfers that data to the appropriate SSF.

The SUI provides the SDP with a list of Site Simulation Files that must be generated. The SDP refers to the DIC files associated with each SSF to determine the exact list of data needed. Because not all sites are completely characterized with site-specific data the SDP is designed to sequentially search the site, regional, and national databases to find a value for the variable. In most cases the SDP simply reads the list of variables from a DIC file and queries the site, regional, national, and chemical databases to either directly transcribe or statistically sample a value for the variable (Figure 3.9). In many cases however, the SDP must process the data found in the master databases. For example, in populating the vadose zone module SSF the SDP must read the value of the vadose zone thickness (VadThick) from the site database and then calculate the value of “dispersivity” based on the following expression :

$$\text{Dispr} = 0.02 + (0.022 \times \text{VadThick})$$

Thus, the SDP represents a sophisticated data extraction and data processing capability within the 3MRA modeling system.

For each **Chemical**
 For each **Site**
 For each **Source Type**
 For each **Waste Level**,

- Specify site layout and transfer all information from the Site Variable Distribution Database to SSF.
- For each variable that has not been defined in the Site Database, transfer all constant variables and stochastic variables (distributions with mean, variance, and range) information, based on the scenario definition (including chemical information for all available chemicals), from the regional statistics database to SSF.
- For each variable that has not been defined in the Site and Regional Database, transfer all constant variables and stochastic variables (distributions with mean, variance, and range) information, based on the scenario definition (including chemical information for all available chemicals), from the National Database to SSF.

End loop on **Waste Level**
 End loop on **Source Type**
 End loop on **Site**.
 End loop on **Chemical**

Figure 3.9 SDP Processing Steps

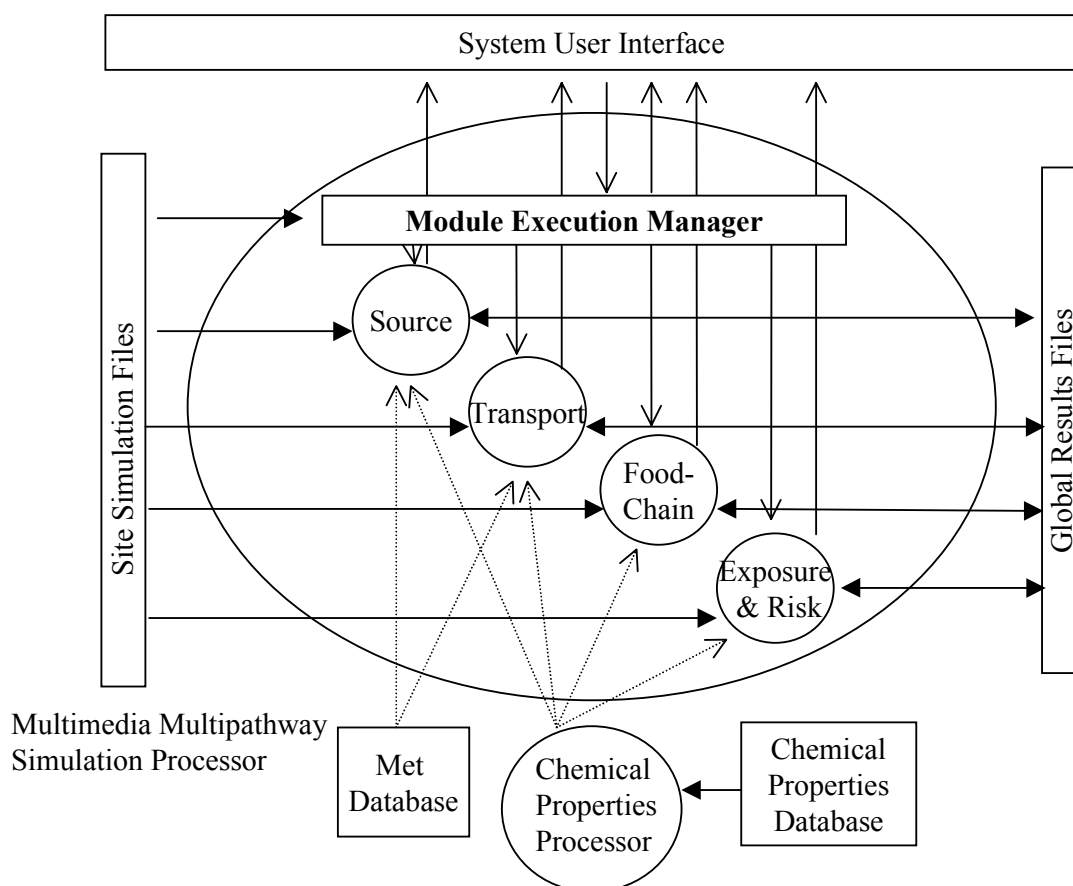


Figure 3.10 Details of the Multimedia Multipathway Simulation Processor
(Dashed lines indicate input from complementary components that are outside the MMSP)

3.3.8 Multimedia Multipathway Simulation Processor (MMSP)

The MMSP represents a software system embedded within a larger software system. The MMSP can be viewed as a site-scale multimedia modeling system, or domain, contained within a national scale regulatory risk assessment methodology, or assessment domain. The primary purpose of the MMSP is to manage the ordered execution of the 3MRA science modules for each site-based assessment requested by the user via the System User's Interface. Management tasks that the MMSP executes include :

- Read input from the Header Site Simulation File (hd.ssf), that contain data that informs the MMSP concerning the site assessment to be conducted and the location of all relevant files and databases.
- Pass necessary simulation data to science modules and invoke their execution in proper sequential order.
- Direct the disposition of intermediate data files produced and consumed within the sequential execution of the science modules. The disposition of the data files

depends on storage options selected by the user and passed to the MMSP by the SUI.

- Terminate processing of science modules and return control to the SUI, reporting any errors that occurred during simulation.
- Provide information on the time elapsed for the processing of each science module.

Figure 3.10 illustrates the MMSP design. The key feature of this design is that the MMSP Execution Manager functions as an interface between the System User Interface (SUI) and the individual science modules. In this capacity the MMSP is invoked by the SUI and provided all information necessary to coordinate a single execution of the science modules. Following structured design techniques, and in particular, the concept of separation of concerns in the software context, the MMSP is not aware of the larger national assessment context within which individual site assessments are conducted. The SUI simply hands control over to the MMSP and waits for the MMSP to return control. The following section describes the MMSP interactions with the science modules.

3.3.8.1 MMSP Science Module Design Features

A science module simulates, in an integrated fashion, a set of environmental processes (physical, chemical, and biological) and in particular, within the 3MRA modeling system, how these processes interact to bring chemical contaminants into contact with human and ecological receptors. In simulating human and ecological risk the 3MRA takes a comprehensive approach to representing the environmental media and processes that play a role. In terms of the software system design for expressing this comprehensive science-based approach the 3MRA applies modern software engineering design principles. In particular, the 3MRA design for the environmental modeling capability centers around establishing modeling components that reflect real world objects. Thus, within the context of site-scale risk assessment such objects include the waste management unit, the watershed, the ecological habitats and associated species home ranges, surface waters (lakes, streams, wetlands), etc. Within the 3MRA, the integrated science of environmental processes is expressed through a total of seventeen individual modules, each simulating a well bounded real world component of the complete environmental risk system. The collection of 3MRA science modules and their relationship as represented in 3MRA is shown in Figure 3.11. The following sections describe the science modules operational characteristics within the larger 3MRA modeling system.

The MMSP design and implementation require that each science module obtain input from specified SSF Data Groups and, possibly, specified GRF Data Groups. Science modules use the IOdll subroutines to read all SSF and GRF Data Groups. The MMSP Module Execution Manager provides each science module with the file name and location of the input data it requires in the SSF and potentially in the GRF Data Groups. Two exceptions to this provision are the meteorological data and, or some science modules, the chemical properties data. If a science module needs meteorological data (observations of wind speed, direction, and stability over a defined time period), that science module is expected to read the Met database using “legacy” methods designed and implemented in previous efforts by EPA. If the module requires chemical properties data that are not provided through an SSF or GRF, the module is expected to use the Chemical Properties Processor to read from the Chemical Properties Database.

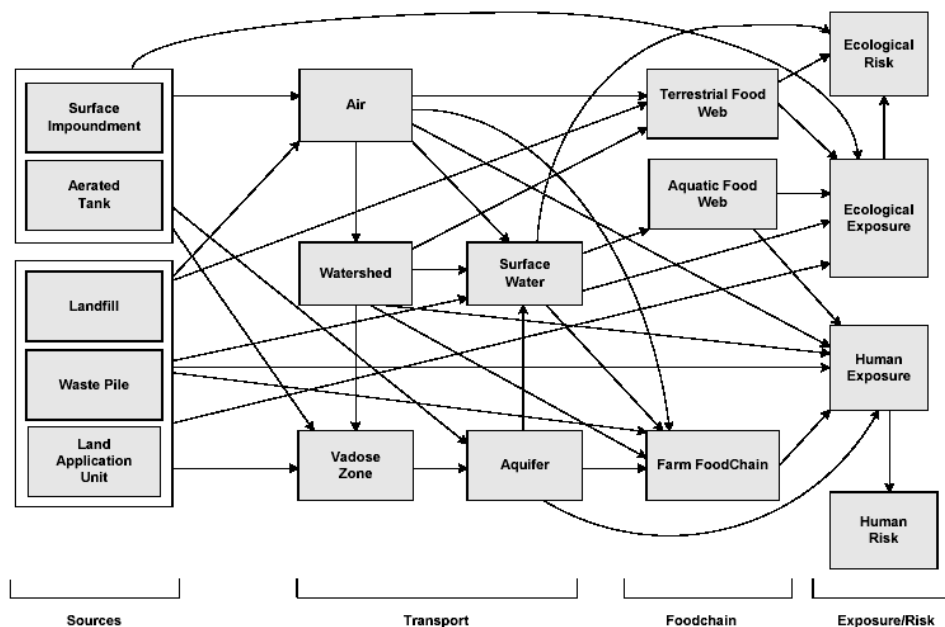


Figure 3.11 Interactions Within the Multimedia Multipathway Simulation Processor

3.3.8.1.1 Science Module Execution

Science modules representing each of the components of the risk assessment process were formulated independently from one another and the system itself. This was possible because all input/output requirements were specified before model formulation occurred. Thus, each module developer knew exactly what data would be input and output from the module (and in what format). Although the MMSP Module Execution Manager guides the sequence of execution and provides the modules with names and locations of input files, the science modules operate as *black boxes* in the MMSP. Thus, these modules do not require the MMSP to provide additional information on how to execute them.

Some of the modules used for the MMSP incorporate legacy models, that is, models that were developed for previous applications outside of the 3MRA context. To incorporate a legacy model the module developer is expected to reformat and reorder data to meet the specific needs of their science module. The reformatting and reordering of data within a computational module can be done by one of three methods:

1. Use pre-processors and/or post-processors without modifying the legacy model.
2. Modify the legacy model to directly read specified files using shared subroutines.
3. Use a combination of processors and model modifications.

These options are shown in Figure 3.12. Note if pre- or post-processors are created for a computational module, a *batch* file also is required as part of the computational module. This batch file serves as the single entry point for execution of that computational module.

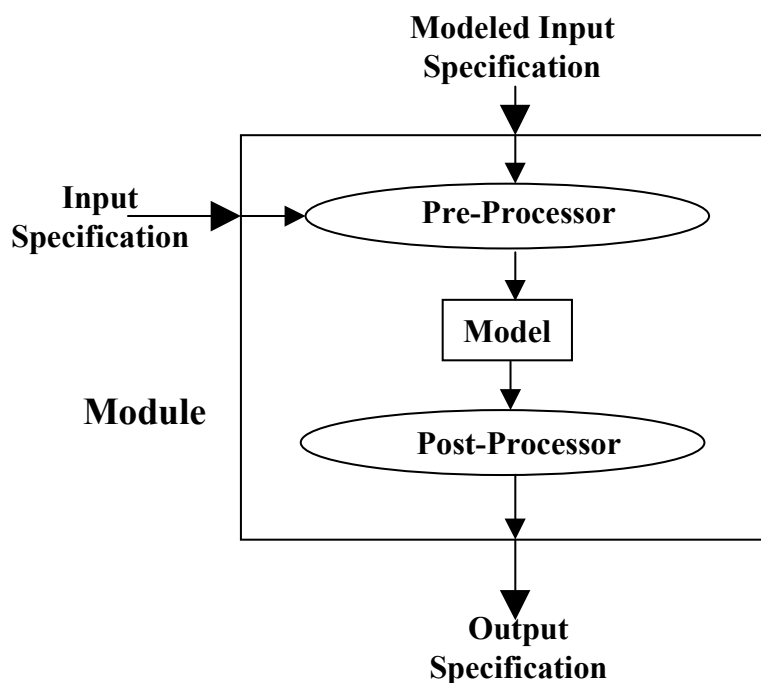


Figure 3.12 How Legacy Models Connect with the FRAMES-HWIR Technology Software System

3.3.8.1.2 Science Module Output

The primary output of the 3MRA science modules are the Global Output Files (GRFs). The GRFs contain the results of the module simulation in a standard format that can be read by other 3MRA modules. A single GRF file is produced by each of the 3MRA science modules. The modules may produce “non-standard” files as well. These files are not recognized by the 3MRA system and generally reflect either data files generated to facilitate the testing of a module or, in the case of legacy models, data files associated with the original legacy outputs. In either case, these files are not used by the 3MRA modeling system.

The MMSP is designed to allow for varying degrees of output storage, addressing varying degrees in quantity (that is, temporary versus permanent files). With a data storage level of zero, the MMSP Module Execution Manager does not copy anything to permanent space and will, delete any temporary files the computational module might have created during its execution. If a computational module is given a data storage level greater than zero, the computational module is responsible for determining what files in addition to the GRF are saved. If a computational module leaves a file in temporary space and the data storage level is greater than zero, the MMSP Module Execution Manager copies that file into permanent space.

3.3.9 The Exit Level Processors (ELP I, ELP II, RVP)

The 3MRA modeling system contains three processors that collectively accumulate, transform, and present information generated by the individual site-based risk assessments. The final outputs of the system are in the form of measures of site and population protectiveness at

the national level. These measures of protectiveness are presented as a function of several modeling dimensions that represent regulatory decision factors, including receptor type, cohort, exposure pathway, chemical, chemical concentration in the wastestream, waste management unit type, and distance from the source.

The Exit Level Processor I (ELP I) reads individual site-based human-health risk/hazard and ecological hazard results from the human and ecological risk modules Global Results Files (hr.grf, er.grf), transforms the population counts into percentages of receptor populations protected, and stores the resulting risk/hazard information in a series of national Risk Summary Output Files (RSOFs). The ELP II and RVP processors query the RSOF in response to specific regulatory criteria for protectiveness and produce graphical and tabular views of the trade off between levels of chemical concentration in wastestreams and levels of protectiveness. With the combination of the RSOF database and the ELP II/RVP a regulatory analyst can ask the following type of question “What is the maximum allowable constituent concentration for wastestreams entering landfills such that at least 90% of all receptors at 95% of the sites nationwide incur a risk less than 10^{-6} ?” The next two sections provide a description of the exit level processors and the risk visualization processor.

3.3.9.1 Exit Level Processor I (ELP I)

The primary role of the ELP I is to prepare a Risk Summary Output File (RSOF). The RSOF is similar to the risk module output file in that it contains a series of cumulative frequency histograms. However, the ELP I converts the contents of histograms from population counts to percentage of population “protected” at each risk level. In addition, the ELP I accumulates the percentage of population protected across all sites and simulations. The end result is an RSOF database that can provide statistics on the percentage of receptors protected nationwide and the percentage of sites that are protected. The RSOF, however, can not discriminate among specific sites. Because the statistics are aggregated over all sites it is not possible, looking in the RSOF, to determine which sites, for example, incur the highest risk.

Table 3.4 lists the dimensions associated with human health risk/hazard before and after the ELP I. A similar set of dimensions for ecological hazard quotients is included in 3MRA (but not shown here). For each combination of dimensions an associated histogram (as shown in Table 3.5). Most significantly, the ELP I eliminates the dimension associated with the number of sites.

In the process of accumulating risk data across sites the ELP I converts the data from population counts per risk/hazard bin into percentages of population incurring less than or equal the risk/hazard associated with the bin. Table 3.6 describes the ELP I processing in matrix form and explains the computational method used to construct the RSOF. There is one matrix for each combination of assessment dimensions shown in Table 3.4. Thus, for a chemical, waste management unit, receptor type, cohort, exposure pathway, Cw, and risk/hazard bin number the matrix shows whether various percentages of the receptor/cohort population are protected at the individual site. For example, the first row in Table 3.6 represents the results for Site#1, Monte Carlo iteration #1, and any single combination of Cw, Risk bin, receptor, cohort, exposure pathway, and waste management unit. For this combination the data in the first row shows that at least 50% of the receptor/cohort population experiences risks less than the particular risk level associated with the bin (it could be any one of the seven risk bins). The next entry in row 1 is a zero (in the cell marked 75%). This means that at this site the percentage of the receptor/cohort population that is protected is not as great as 75%, or, said differently, more than 25% of the

receptor/cohort population is not protected. When a column is summed the total value represents the number of sites (and therefore the percentage of all sites) for which the column labeled percentage of receptor/cohort population is protected. This total is contained in the last row of Table 3.6 and is the only data from the matrix to be stored in the RSOF (all rows associated with individual sites are released). Table 3.7 shows the unit matrix stored in the RSOF. For each assessment dimension shown in Table 3.4 there is a Table 3.7 in the RSOF. The table lists the waste concentration levels (Cw's) versus individual bin levels of risk/hazard. In each cell is an array of ten values, each reflecting a total count across all site simulations that resulted in the specified percentage of the population being protected.

Table 3.4. Summary of Parameter Requirements Associated with Human-Health Risk/Hazard for the ELP-I

Parameters	Dimensions	
	Supplied by Human-Risk Module	Stored by ELP-I and Provided to RVP
Number of Distances ^(a)	3	3
Number of Exposure Pathways plus Summation of Pathways ^(b)	12	12
Number of Receptor Types plus Summation of Receptor Types ^(c)	16	5
Number of Cohorts plus Summation of Cohorts ^(d)	5	4
Number of Bins to Tally Individual Excess Cancers ^(e)	7	7
Number of Bins to Tally hazard Quotients (Non-Cancer) ^(f)	4	4
Number of Critical Year Percentiles ^(g)	1	1
Number of C _w s ^(h)	5	5
Number of Chemicals ⁽ⁱ⁾	40	40
WMU Types ^(j)	5	5
Number of Sites/WMU-Type Combinations ^(k)	419	---
Percentiles of Protected Population ^(l)	---	10

(a) "n" distance rings are designed into the ELP-I, but only three distances are stored for HWIR calculations: 0 to 0.5 km, 0 km to 1 km, and 0 to 2 km from the edge of the waste site area.

(b) Inhalation Air, Inhalation through Showering, Summation of all Inhalation Pathways, Ingestion of Groundwater, Ingestion of Soil, Ingestion of Meat, Ingestion of Milk, Ingestion of Fish, Ingestion of Breast Milk, Ingestion of Vegetables, Summation of all Ingestion Pathways, Summation of all Inhalation and Ingestion Pathways.

(c) The risk module analyzes 16 receptor types (8 each with and without drinking water): Beef Farmer, Dairy Farmer, Beef Farmer Fisher, Dairy Farmer Fisher, Gardener, Gardener Fisher, Resident, and Resident Fisher. Of these 16 receptor types, the risk module rolls-up the results and passes only 5 receptor types to the ELP-I:

Beef/Dairy Farmer, Gardener, Fisher, Resident, and Summation of Receptor Types.

(d) The risk module analyzes five cohorts: Infants, 1-6 years old, 7-12 years old, 13-17 years old, and 18 years old and older (adult). Risk information on the five cohorts is passed to the ELP-I, where the ELP-I rolls-up the information into four cohorts: Infants, 1-12 years old, 13 years old and older (adult), and Summation of all Cohorts.

(e) Risk bins include $(0.0 - 5.0 \times 10^{-9})$, $(5.0 \times 10^{-9} - 7.5 \times 10^{-8})$, $(7.5 \times 10^{-8} - 7.5 \times 10^{-7})$, $(7.5 \times 10^{-7} - 2.5 \times 10^{-6})$, $(2.5 \times 10^{-6} - 7.5 \times 10^{-6})$, $(7.5 \times 10^{-6} - 5.0 \times 10^{-5})$, and $>5.0 \times 10^{-5}$. Each risk bin for human health stores by Chemical and WMU type the **Number of Sites** that protects at least some percentage of the human population (0%, 5%, 25%, 50%, 75%, 85%, 90%, 95%, 98%, or 99%) for each "risk-bin/ C_w " pair by distance, pathway, receptor, cohort, and critical-year method.

(f) Hazard bins include $(0.0 - 0.05)$, $(0.05 - 0.5)$, $(0.5 - 5.0)$, and >5.0 . Each hazard bin for human health stores by Chemical and WMU type the **Number of Sites** that protects at least some percentage of the human population for each "hazard-bin/ C_w " pair by distance, pathway, receptor, cohort, and critical-year method.

(g) The critical year is defined as the year associated with a risk representing a percentage of the peak

(h) Five levels of C_w before disposal are stored (mg/L for waste water [SI and AT], mg/kg dry weight for solids [WP and LF], and mg/kg wet weight [LAU]). These levels are chemical specific.

(i) Although the actual number of chemicals assessed per production run varies, the ELP-1 was designed to at least address 40 chemicals, where 40 chemicals represent a subset of the total number of chemicals to be assessed, as part of HWIR.

(j) WP, LAU, SI, AT, and LF.

(k) Each site may contain multiple WMU types, but each WMU type will be assessed one at a time. The maximum possible number of possible combinations is 419, as some sites may not contain a particular WMU type.

(l) Currently, 10 population protection percentiles have been identified: 99%, 98%, 95%, 90%, 85%, 75%, 50%, 25%, 5%, and 0%. These percentiles represent the percentage of the population that at least has been protected. For 90%, for example, at least 90% of the population has been protected.

Table 3.5. Summary of Human Risk Bins and Labels

Risk Bin Number	Risk Bin Range	Risk Bin Label
1	$0.0 \leq X < 5 \times 10^{-9}$	1×10^{-9}
2	$5 \times 10^{-9} \leq X < 7.5 \times 10^{-8}$	1×10^{-8}
3	$7.5 \times 10^{-8} \leq X < 7.5 \times 10^{-7}$	5×10^{-7}
4	$7.5 \times 10^{-7} \leq X < 2.5 \times 10^{-6}$	1×10^{-6}
5	$2.5 \times 10^{-6} \leq X < 7.5 \times 10^{-6}$	5×10^{-6}
6	$7.5 \times 10^{-6} \leq X < 5 \times 10^{-5}$	1×10^{-5}
7	$5 \times 10^{-5} \leq X$	1×10^{-4}

Table 3.6. Procedure to Compute a Risk Summary Output File

C_{wi} and Risk/Hazard Bin_j^(a)											
Index on Site (1 to N sites)	Index on Iteration (1 to M iterations)	Equal To or Greater Than Percentage of Population Protected									
		0%	5%	25%	50%	75%	85%	90%	95%	98%	99%
1	1	1 ^(b)	1	1	1	0	0	0	0	0	0
2	1	1	1	1	1	1	1	1	0	0	0
N	1	1	0	0	0	0	0	0	0	0	0
1	2	1	1	1	0	0	0	0	0	0	0
2	2	etc.									
N	2										
1	M										
2	M										
N	M										
Sum of Counts by Column ^(c)		Column 1	Column 2	Column 3	Column 4	Column 5	Column 6	Column 7	Column 8	Column 9	Column 10

(a) “i” is the index on the C_w from one to five, and “j” is the index on the Risk/Hazard Bin. For human risk, there are seven excess cancer bins; for human hazard, four hazard quotient bins; for ecological hazard, five ecological-hazard quotient bins. A similar table is associated with each “ C_w &risk/hazard bin” pair.

(b) For each site and iteration combination that meets the population-protection criterion, the cell is assigned a value of unity, representing protection. When the cell does not meet the population-protection criterion, the cell is assigned a value of zero, representing no protection.

(c) The ELP-1 only stores cumulative counts by column in the RSOFs (that is, last row of Table 3.6).

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Table 3.7 Example ELP I Output Table

C _w	Risk/Hazard Bin				
	1	2	3	M
1	C(1,1) _i	C(2,1) _i	C(3,1) _i		C(M,1) _i
2	C(1,2) _i				
3	C(1,3) _i				
N	C(1,N) _i				C(M,N) _i

M = Number of Risk/Hazard Bins

N = Number of C_ws

C = Summation of counts per percentage of population protected

i = index on the percentage of population protected (i.e., 0%, 5%, 24%, 50%, 75%, 85%, 90%, 95%, 98%, 99%)

3.3.9.2 Exit Level Processor II (ELP I) and Risk Visualization Processor (RVP)

As described in Section 2 the overall objective of the 3MRA national assessment methodology is to assess the potential human and ecological risks resulting from the disposal of industrial wastestreams in land-based waste management units. It is of interest to regulatory decision analysts to know the quantitative relationship between constituent concentration levels and national risk (or hazard in the case of non-carcinogenic chemicals). National risk is expressed in 3MRA in terms of two measures of protectiveness, percentage of the national population experiencing risks less than an assigned regulatory threshold and the percentage of sites where a regulatory established percentage of the local population experiences risks less than an assigned regulatory threshold. For example, regulatory decision analysts may wish to know a concentration level for benzene that if applied to all wastestreams (i.e., any wastestream exceeding this concentration of benzene would require disposal as a hazardous waste in a Subtitle C waste management unit and any wastestream with a lesser concentration of benzene would be allowed disposal in a Subtitle D waste management unit), in all geographic locations, regardless of the type of waste management unit, would result in at least 95% of the population at 99% of the sites experience excess cancer risks less than 10^{-6} .

The Risk Summary Output Files (RSOFs) generated by the ELP I contain the necessary data to allow the ELP II and RVP to calculate specific constituent concentration levels that satisfy the regulatory decision criteria related to policy-based protection percentages (population and sites) and risk thresholds.

The following sections provide a description of the means by which the ELP II and the RVP facilitate the analysis and selection of national exit levels.

The RVP and ELP II actually share the software that performs the protection-based calculations, as requested by the user. The difference between the RVP and the ELP II is solely in how they output the results. The RVP is invoked from within the ELP II and provides the regulatory analyst a menu driven user interface for specifying protection and risk criteria and viewing graphically the resulting relationship between constituent concentration levels, protection criteria, and risk thresholds. The ELP II provides the ability to calculate national exit levels as a function of the regulatory decision criteria. Figure 3.13 illustrates the RVP and ELP II use of the Risk Summary Output Files (RSOFs) generated by the ELP I to produce the graphical and tabular views of the relationship between constituent concentration levels and population/site protectiveness.

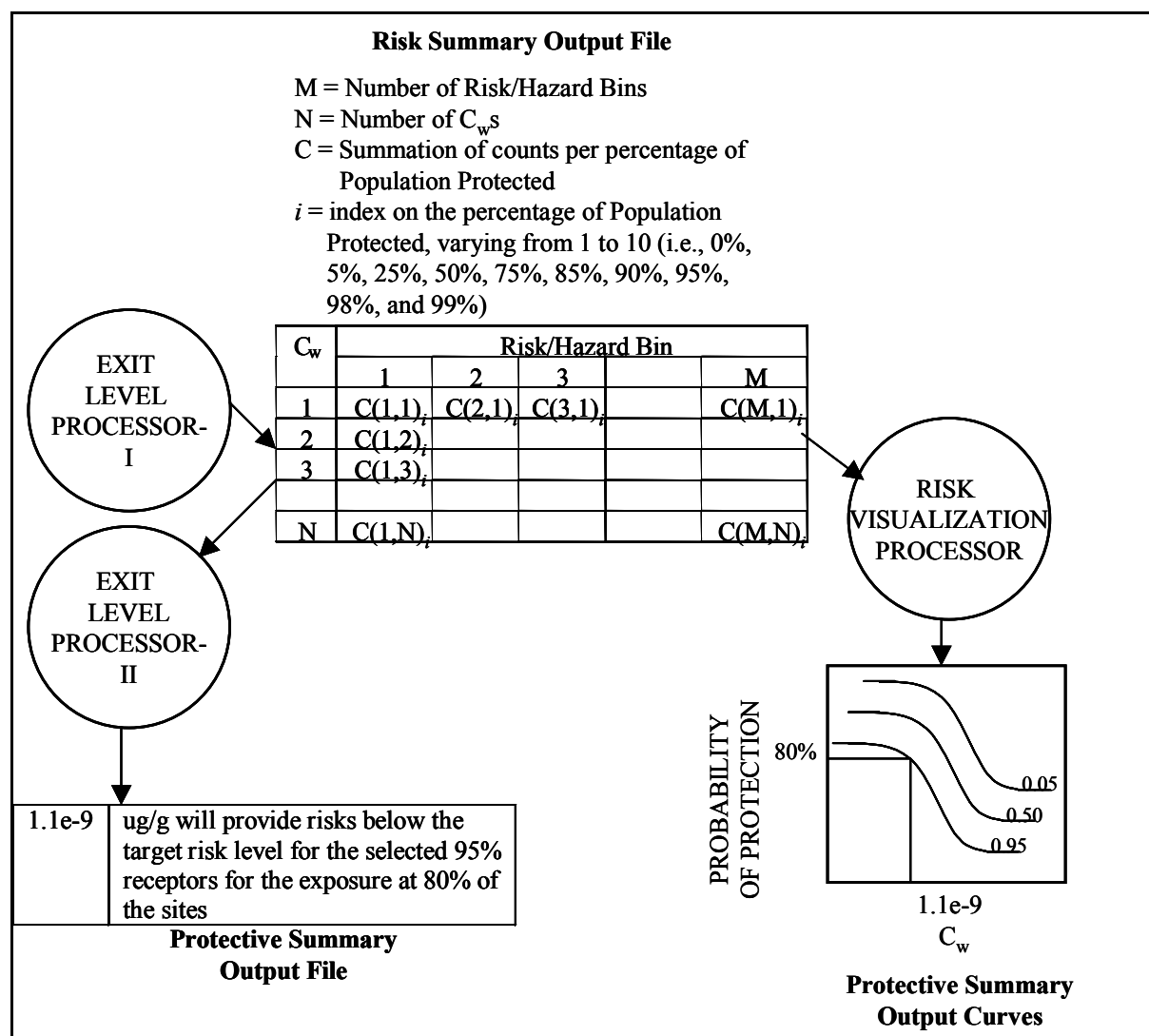


Figure 3.13 Relationship among ELP I, ELP II, and RVP

Both the RVP and the ELP II allow the regulatory analyst to apply the decision criteria to risk and hazard data as a function of the assessment factors listed in Table 3.4. Thus, the regulatory analyst can view risk and hazard information for human and ecological receptors from several perspectives.

Graphical View of Protectiveness vs C_w

The RVP allows the user (e.g., regulatory decision analyst) to query and summarize the information stored in the RSOFs and to graphically view the results of such queries. The user provides a set of assessment factors (i.e., WMU type, chemical, distance, receptor type, cohort, etc.) and a level of protection (for example, risk of 1.0×10^{-6} or HQ of 1.0, etc.). The RVP uses this information to construct plots showing the probability of protecting specified percentages of human or ecological receptors as a function of C_w .

The RVP retrieves data from the RSOFs, generates a plot of probability of protection as a function of C_w , and displays this plot on the screen. Figures 3.14 and 3.15 illustrate the human risk protective summary and ecological hazard protective summary plots produced by the RVP, respectively.

The probability of protection (y-axis) represents the probability that any given site is protective, or, the percentage of sites found to be protective under the various values of C_w (x-axis) and for specified percentages of the receptor/cohort population (individual curves). Each plot is generated for a set of user selected assessment factors (shown in the right hand side of the Figures). The decision analyst can vary the assessment factors and decision criteria and quickly determine the change in the C_w vs probability of protection relationship.

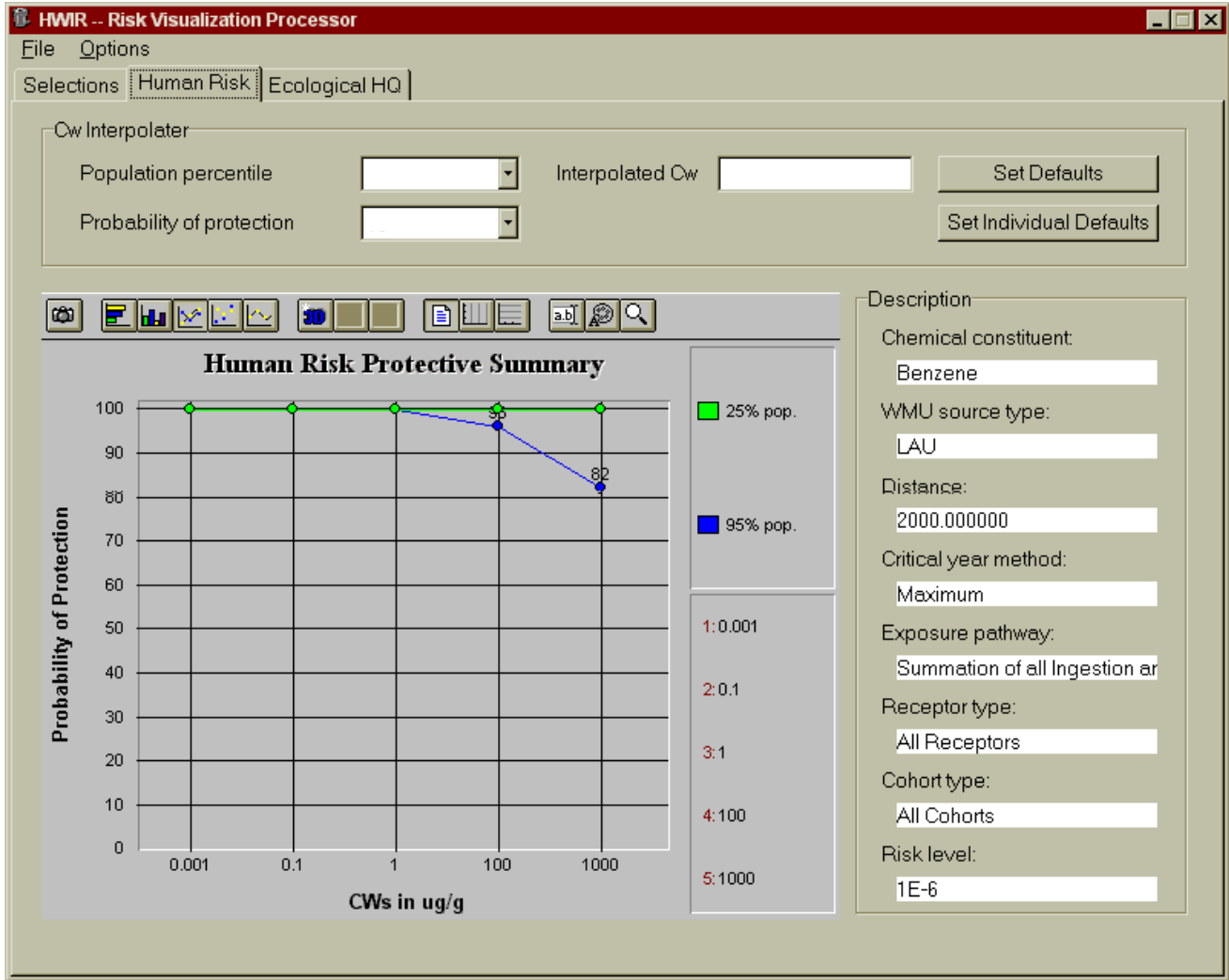


Figure 3.14 Protective Summary Output Figure for Human Risk

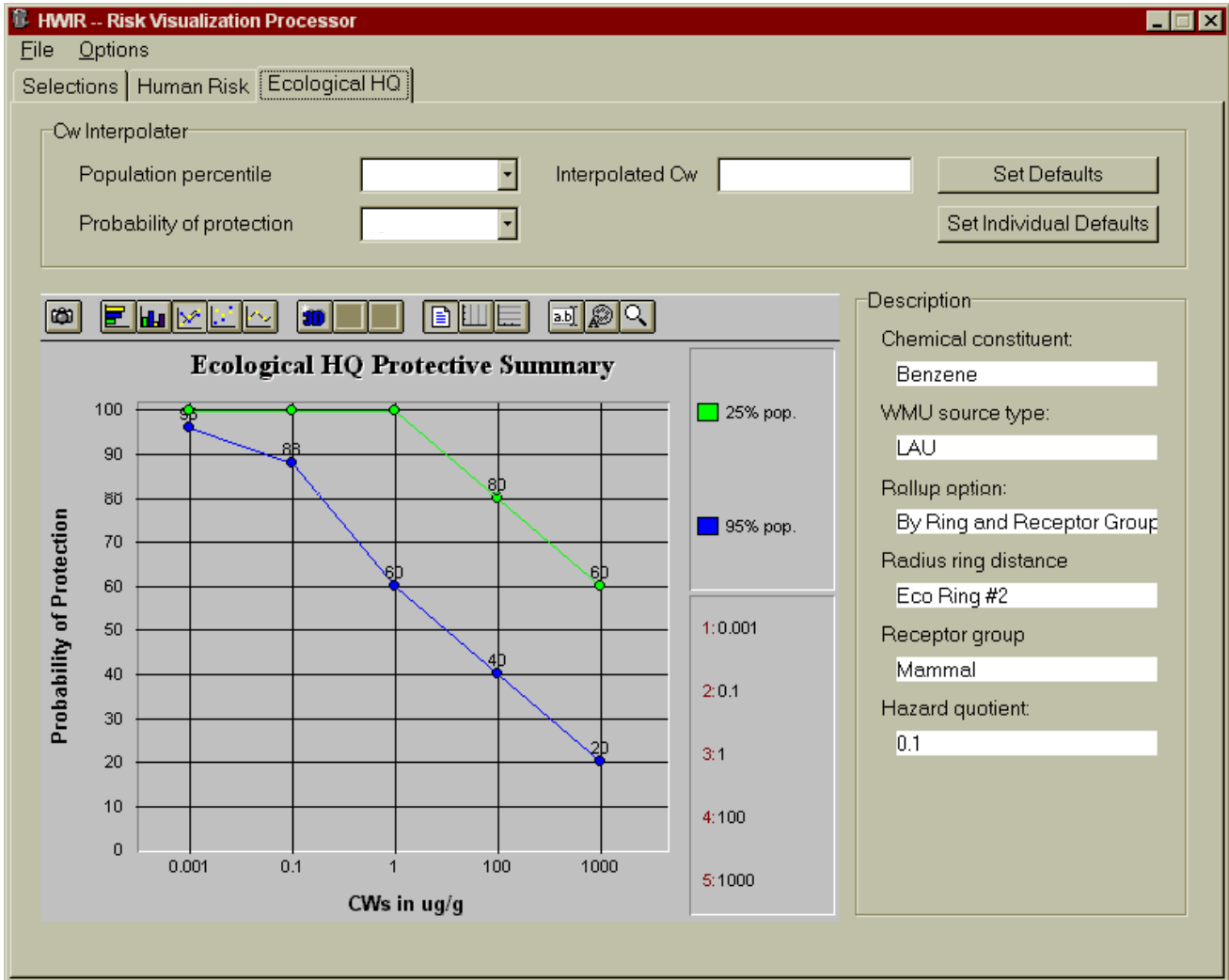


Figure 3.15 Protective Summary Output Figures for Ecological HQ

Tabular View of Protectiveness vs Cw

The ELP II consumes and processes RSOF-based data with the same software used by the RVP. The ELP-II assesses five scenario options and generates seven types of tables and places them in the Protective Summary Output Files (PSOFs). A scenario table, such as is shown in Table 3.8, is created to store the scenario and default selections (representing regulatory criteria). A scenario is defined to include three risk/hazard thresholds (Human Risk, Human Health Hazard Quotient, and the Ecological Hazard Quotient), probability of protection, and a population-percentile. Other scenario descriptors for human health include distance, exposure pathway, receptor type, cohort, critical-year method. Other descriptors for ecological health include distance, and habitat group, habitat type, receptor group, and trophic level for ecological risk.

Table 3.8 3MRA Regulatory Scenarios

SCENARIO ^(a)	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
Risk Level	10 ⁻⁶	10 ⁻⁶	10 ⁻⁵	10 ⁻⁵	10 ⁻⁷
Human Health-HQ	1	1	1	10	10
Ecological-HQ	1	1	1	10	10
Population-Protection Percentile	99	99	99	95	98
Probability of Protection	95	85	85	85	90
(a) When comparing scenarios, the remaining scenario parameters (for example, exposure pathway, receptor type, etc.) do not change from scenario to scenario and, therefore, are not presented in this table. The parameters shown in the table can be changed by the user on subsequent executions of the ELP II.					

Seven types of tables are created by the ELP-II in the PSOF directory. The following tables use the exit level scenario settings created in the RVP/ELP-II user interface to produce the desired results. The tables generated here reference “exit levels”. This term is specific to a particular regulation entitled the Hazardous Waste Identification Rule (HWIR). The HWIR focused on defining Cw’s that represent thresholds between hazardous and non-hazardous waste classifications. Other regulatory programs may present ELP II output data in a different format but the basic data processing of the ELP I and ELP II would remain the same.

Lowest Target Exit Level tables are quantitative criteria for allowing a specific class of industrial waste streams to no longer require disposal as a hazardous waste (that is, to *exit* Subtitle C) and to allow disposal in Industrial Subtitle D facilities. Hazardous waste constituents with values less than these exit-criteria levels would be reclassified as nonhazardous wastes under the Resource Conservation and Recovery Act. In these tables, the lowest exit level

concentrations for human health (that is, human risk and hazard) and ecological hazard will be evaluated and reported.

Table 3.9 Example Lowest Target Exit level Concentrations

Chemical	CasId	Liquid			Semi-Solid			Solid			Landfill			Other WMU...		
		HH	Eco	Lowest	HH	Eco	Lowest	HH	Eco	Lowest	HH	Eco	Lowest	HH	Eco	Lowest
Benzene	71-43-2	4.00E-01	3.00E+01	4.00E-01												
Lead	7439-92-1	1.00E-05	3.00E+01	1.00E-05												

The Target Exit Level table summarizes the results contained in the Lowest Target Exit Level tables for each chemical and WMU type by recording the lowest target exit level concentration from all categories (human health and ecological hazard) and assigning that one value to its respective scenario. Therefore, each chemical, WMU type, and scenario will be assigned one target exit level concentration (that is, the lowest associated with that scenario). In addition, this table will note whether the lowest target exit level concentration was based on the maximum C_w used in the assessment.

Table 3.10 Example Target Exit level Concentrations by Scenario

Chemical Name	CasId	Scenario 1	Max Used	Scenario 2	Max Used	Other Scenarios...
Benzene	71-43-2	4.00E-01	“no”	1.00E+02	“no”	
Lead	7439-92-1	1.00E-05	“no”	1.00E-04	“no”	

Relative Target Exit Level tables give the ratio between the first scenario’s (that is, Scenario 1 in Table 2.1) target exit level identified and the target exit level of each other scenario for each WMU type.

Table 3.11 Example Relative Target Exit Level Concentrations

Chemical Name	CasId	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
Benzene	71-43-2	1	2.00E+02	3.00E-02	3.00E+00	3.00E+00
Lead	7439-92-1	1	1.00E+01	1.00E+00	1.00E+00	1.00E+00

50% Probability of Protection tables are similar to the Target Exit Level tables; however, the probability of protection for each scenario is set to 50%.

Table 3.12 Example Target Exit Level Concentrations, Based on 50% Probability of Protection

Chemical Name	CasId	Scenario 1	Max Used	Scenario 2	Max Used	Other Scenarios...
Benzene	71-43-2	1.00E+02	“no”	1.00E+02	“no”	
Lead	7439-92-1	1.00E-04	“no”	1.00E-04	“no”	

Cohort Human Risk/HQ table contains the risk trigger levels found associated with the Protective Summary Output curves for each cohort category, WMU type, and waste type. In effect, target risk/hazard level (for example, 10^{-6} for risk and 1.0 for human HQ) is determined as a function of an exit level concentration by cohort category. The previous tables have computed the target exit level concentration as a function of the target risk/hazard level.

Table 3.13 Example Cohort Human Risk/HQ for Landfill

Chemical Name	CasId	Landfill					
		Infants		1–12 years old		13 years old and older	
		Risk	HQ	Risk	HQ	Risk	HQ
Benzene	71-43-2	1E-04	NA	8E-07	NA	0.000005	NA
Lead	7439-92-1	1E-04	NA	0.0001	NA	0.0001	NA

Receptor Human Risk/HQ table contains the risk trigger levels found associated with the Protective Summary Output curves for each receptor category, WMU type, and waste type. As with the Cohort Human Risk/HQ tables, the target risk/hazard level is determined as a function of an exit level concentration by receptor category.

Table 3.14 Example Receptor Human Risk/HQ for WP

Chemical Name	CasId	WP							
		Beef/Dairy Farmer		Gardener		Fisher		Resident	
		Risk	HQ	Risk	HQ	Risk	HQ	Risk	HQ
Benzene	71-43-2	4E-08	NA	0.000003	NA	0.000006	NA	8E-07	NA
Lead	7439-92-1	0.0001	NA	0.0001	NA	0.0001	NA	0.0001	NA

Exposure Pathway Human Risk/HQ table contains the risk trigger levels found associated with the Protective Summary Output curves for each exposure category, WMU type, and waste type. As with the Cohort Human Risk/HQ tables, the target risk/hazard level is determined as a function of an exit level concentration by exposure pathway category.

Table 3.15 Exposure Pathway Human Risk/HQ

Chemical Name	CasId	Air Inhalation		Soil Ingestion		Water Ingestion		Crop Ingestion	
		Risk	HQ	Risk	HQ	Risk	HQ	Risk	HQ
Benzene	71-43-2	0.000006	NA	2E-09	NA	1E-04	NA	0.00002	NA
Lead	53-70-3	1E-04	NA	0.0001	NA	1E-04	NA	0.0001	NA