
API'S DECISION SUPPORT SYSTEM FOR EXPOSURE AND RISK ASSESSMENT (DSS)

VERSION 2.0

HEALTH AND ENVIRONMENTAL SCIENCES DEPARTMENT
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Health and Environmental Sciences Department

API PUBLICATION NUMBER 4685

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MARCH 1999



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API DSS QUICK START SHEET

Before calling Technical Support, please review the following document to see if your question is addressed.

Hardware and Software Requirements

The API DSS requires the following configuration:

- An Intel® 486 (with math coprocessor) or any 100%-compatible machine
- Windows® 3.1, NT, 95®, or 98®
- At least 8 megabytes of RAM
- At least 8 megabytes of free space on the hard-disk drive
- Microsoft EXCEL® version 5.0 for Windows®

Installation Procedure

The following steps will install the DSS on your computer; a new Windows® program group as well as a "API DSS 2.0" icon will be installed into your Windows® desktop. An uninstall option is available under the API DSS program group. The uninstall option will delete the DSS files and directory along with the API DSS icon and group.

For Windows^B 3.1:

Step 1 Insert Distribution Disk #1 in drive A or B.

Step 2 Select "File" from the Program Manager menu and "Run" from the pull-down menu. Enter the following command in the dialog box:

a:\install.exe

Select OK on the Run dialog box.

Step 3 Follow the instructions in the installation package.

For Windows^{95, 98,} and Windows[®] NT:

Step 1 Insert Distribution Disk #1 in drive A or B.

Step 2 Select the "Start" button and then "Run..." from the pop-up menu. Enter the following command in the "Open" dialog box:

a:\install.exe

Select OK.

Step 3 Follow the instructions in the installation package.

Running the DSS

Starting DSS under Windows@8.1:

Double-click on the "API DSS 2.0" icon in the API DSS group.

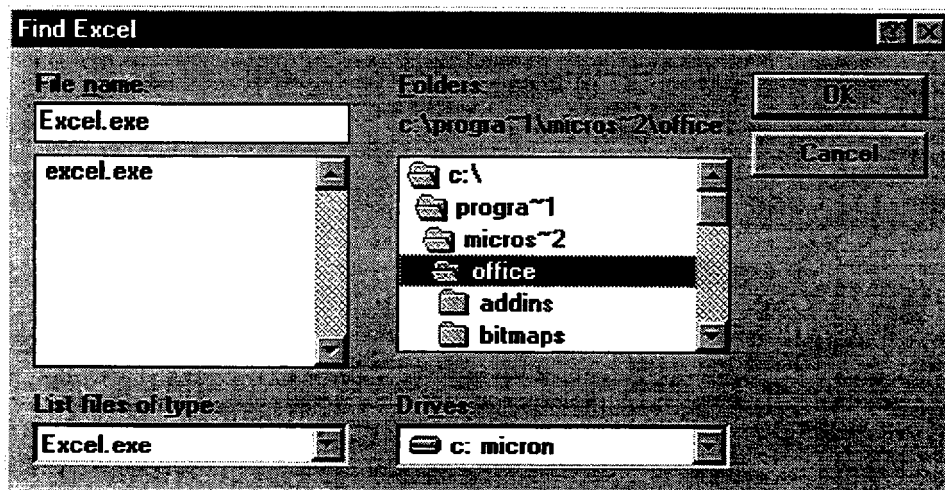
Starting DSS under Windows® 95.98, and Windows@NT:

Double-click on the "API DSS 2.0" icon from the Windows desktop or select "Programs", "API DSS", and "API DSS 2.0" from the Start menu.

Starting the DSS is the only time you need to double-click. Double-clicks are not required from within the DSS software and will be misinterpreted. All **clicking within the DSS must be single clicks**.

Locating EXCEL for the DSS

When the DSS is opened for the first time, the user will be asked to "browse" (using a file menu) to the location where EXCEL@s loaded on their system. Using the file menu shown, the user should change the directory until the file "EXCEL.exe" is shown in the "File name:" box.



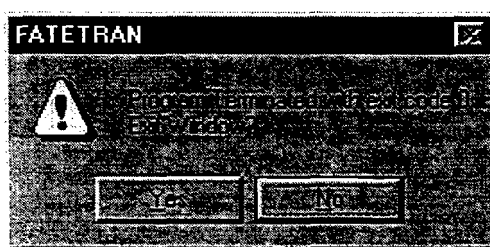
Remember, EXCEL@ may be located on a network drive. Once the location of EXCEL@ has been identified this window will not appear again. If you are unable to locate EXCEL® for the time being, select "Cancel"; you can still use the DSS however you will be unable to bring up the FORTRAN results in EXCEL® automatically. When the DSS is opened the next time it will ask again for the location of EXCEL® (it will do this until the location has been established).

NOTE: If you are unable to locate EXCEL® but can still open EXCEL® from your Windows® desktop, you may run the EXCEL® macros externally from the DSS to view the FORTRAN results.

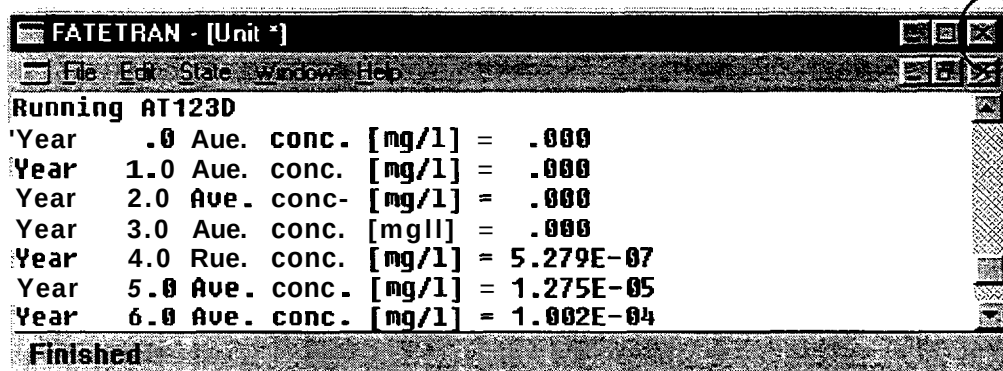
- If you have just run the fate and transport models, open EXCEL® (from your Windows® desktop not the DSS) and open the file called "APIDSSTP.xls".
If you have just run the chemical intake model, open EXCEL® (from your Windows® desktop not the DSS) and open the file called "APIDSSRK.xls".

Running the FORTRAN codes:

Upon successful execution of any of the DSS's FORTRAN models, Windows will display the message, 'Program Terminated with exit code 0. Exit Window?'



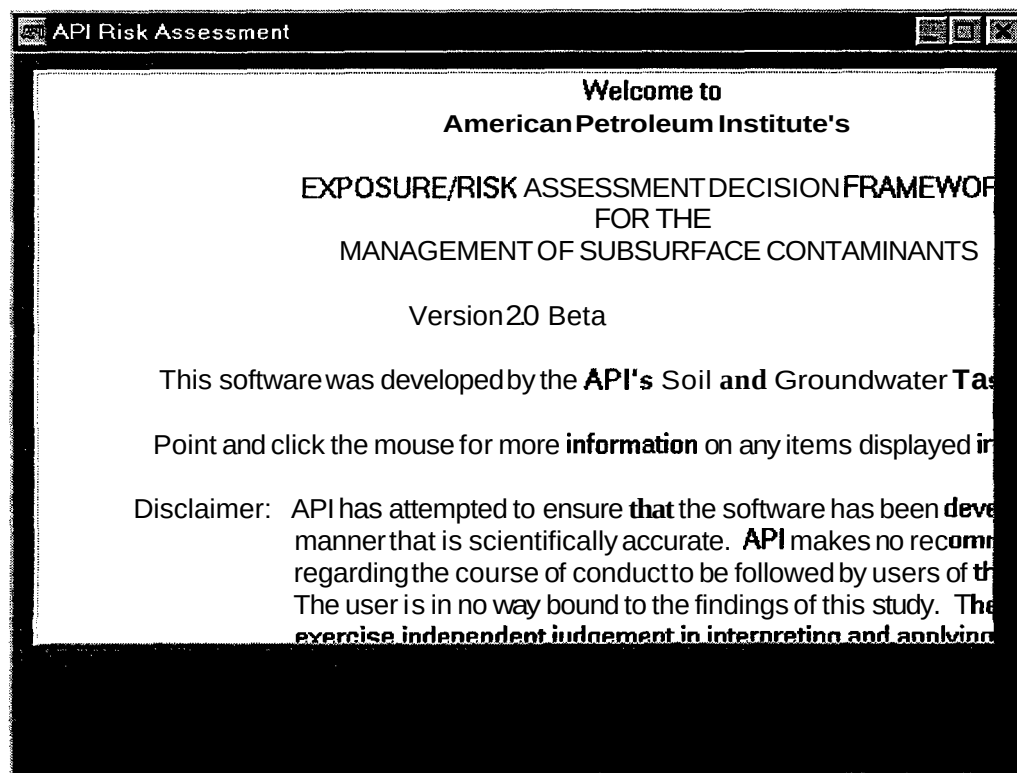
You will be prompted to click on 'Yes' or 'No'. **This is not an error message!** If you click on 'Yes' the FORTRAN runtime window will be closed and you will be returned to the DSS. If you select 'No' you can browse back up through the FORTRAN output (AT123D displays groundwater concentration with time); when you are through, close the FORTRAN runtime window (by selecting "File", "Exit", or double-click on the window control box) and you will be back in the DSS.



Saved Files from Previous Version 1.x

Saved files from previous DSS versions are not compatible with version 2.0. Too many additional features were added (especially in the **SESOIL** inputs) to keep the compatibility option. The easiest way to get the old data into the new version is to print out the "Data Requirements" summary from the previous version and then retype in the data.

If the Initial Screen Looks Like This:



You need to set the "Font" option in your Windows' display panel to "Small Fonts". The API DSS must be run with the small fonts option. To do this, select "Settings" from the Windows Start Menu and then select "Control Panel". Then select "Display". Under the "Settings" tab make sure that "Small fonts" are selected under the "Font Size" option (not "Large Fonts"). Click on the OK button.

EXECUTIVE SUMMARY

The American Petroleum Institute's (API) Exposure and Risk Assessment Decision Support System (DSS) has been developed to assist environmental professionals in estimating human exposure and risk from contaminated sites. The DSS is a valuable, user-friendly tool that can be used to (i) estimate site-specific risks, (ii) identify the need for site remediation, (iii) develop and negotiate site-specific cleanup levels with regulatory agencies, and (iv) efficiently and effectively evaluate the effect of parameter uncertainty and variability on estimated risk.

The API DSS Version 2.0 consists of four modules. The Development of Risk Scenario module allows the user to develop a conceptual model for estimating the risk. The Receptor Point Concentration module allows explicit entry of receptor point concentrations or estimates the **concentrations** by contaminant fate and transport modeling. The fate and transport models included in the DSS are: SESOIL, VADSAT, and Jury unsaturated zone models; AT123D and VADSAT saturated zone models; and Farmer's, Jury's, VADSAT and Thibodeaux's air emission models linked with a box or Gaussian dispersion model. The Chemical Intake and Risk Calculation module uses estimated or user-entered receptor point concentrations to estimate chemical intake by a human receptor for several different exposure routes. Further, this module uses the estimated dose and chemical-specific toxicity (slope factor or potency value for carcinogens and the reference dose for non-carcinogens) to estimate carcinogenic risk and noncarcinogenic hazard index. Finally, the Risk Presentation module allows the user to view the results of the analysis in tabular and graphical formats. The DSS includes databases accessed by the various modules and contains **chemical-specific** fate and transport properties, toxicity properties and default uptake parameters for 86 chemicals. Report-ready tables and graphs depicting the exposure and risk results can be printed.

The Chemical Intake and Risk Calculation module of the DSS can be implemented in either deterministic or Monte Carlo simulation modes. The latter is used to quantify the uncertainty in the exposure and risk results due to uncertainty in the input parameters.

The **DSS** runs under the Microsoft Windows[™] 95, 98, 3.1, or NT environments. It is user friendly and includes online help. The software accesses FORTRAN codes to perform computations and relies on EXCEL[™] spreadsheet software (version 5.0 or higher) to present results in report-ready tabular and graphical formats.

System Limitations

DSS limitations include:

- The maximum number of chemicals for a DSS session is limited to twenty.
- The **DSS** can only consider one receptor at a time. This limitation was imposed to simplify system output and its interpretation. If a user wants to analyze the risk posed to two different receptors, he or she may run the **DSS** twice. Default parameter values from the first analysis can be saved and then retrieved for the second analysis.
- The DSS includes six routes of exposure **as** discussed in Section **6.0**. Other exposure routes such as the ingestion of produce grown in contaminated soil or the inhalation of indoor air in confined spaces (such as basements), are not addressed. Depending on the site-specific conditions, these routes of exposure may be significant.

Other assumptions and limitations include:

- The EPA Uptake Biokinetic model for lead is not included in the software. If lead is added to the **DSS** database, it will be treated in the same manner **as** other chemicals requiring a slope factor or reference dose.
- Risks are additive; chronic effects are additive.
- Risks are carcinogenic only. Teratogenicity, mutagenicity, etc., are not considered.
- Chronic toxicities are not specified **by** toxic effect or affected organ.
- Fate and transport models may assume steady-state and compositional equilibrium between phases at all times.

- Risk is to a **maximally** exposed individual. **Population** risks are not addressed.
- Subchronic risks are not addressed by the DSS. The database does not contain toxicity **values** for subchronic exposures (**less** than two years).
- Risks/chronic effects to **children** can be **calculated** by assuming that a child is a "**small adult**." It is assumed that potency factors, **RfDs**, **apply** to children as **well** as adults.

Differences Between Version 2.0 and 1.0

The **following** additions **and/or** changes to the software have been made in version 2.0:

- The VADSAT **model** was added.
- The new **SESOIL** code (1996) was incorporated and the interface was updated to **allow** the user **full** access to **all** of the **SESOIL** options (except the erosion **module**).
- Monte **Carlo capabilities** were removed for the fate and transport **models**.
- The new AT123D version **developed** by H.S.I. **GeoTrans** (for the EPA) was incorporated. (This version of AT123D corrected a **problem** with the **pulse** source option in the **original** AT123D code.)
- The AT123D coordinate system was changed to make it more intuitive to use.
- The user may now enter time step size for AT123D. Using **smaller** time steps **will help** reduce the number of cases where **oscillations** in the **solution** occurred.
- A new **capability** was added to import concentration-time series data generated by **models** external to the DSS.
- A user interface was added to **allow** users to append or modify the **toxicological** and **physical/chemical** property databases **directly** from the DSS.

1.0 OVERVIEW OF THE DECISION SUPPORT SYSTEM

1 . INTRODUCTION

This section presents an overview of the American Petroleum Institute's (API) Exposure and Risk Assessment Decision Support System (DSS) Version 2.0. The DSS is a valuable user-friendly tool that can estimate risks at sites contaminated by petroleum hydrocarbons and other contaminants. While the DSS is a convenient tool for preparing a relatively complex level of risk assessment, it should be run by personnel knowledgeable in risk assessments.

The ~~exposure~~/risk assessment process is a multidisciplinary process requiring expertise in data collection and site characterization, contaminant fate and transport modeling, toxicology, environmental chemistry, and data analysis. Both federal and state guidance encourage the use of site-specific risk assessments as well as the evaluation of uncertainty in estimated risk (e.g., EPA Risk Assessment Guidance for Superfund and the Texas Risk Reduction Rules). It is important to develop a computerized framework to provide a consistent and cost-effective approach for determining risk and cleanup levels at sites with subsurface contamination. The development of the DSS is a first step in ensuring a consistent approach.

1.2 DESCRIPTION OF THE **RISK** ASSESSMENT PROCESS

As described by the National Academy of Sciences (1983), the risk assessment process consists of four steps: (1) hazard identification, (2) exposure assessment, (3) dose-response assessment, and **(4)** risk characterization. These steps are illustrated in Figure 1-1 and briefly described below. Details are available in EPA (1989a).

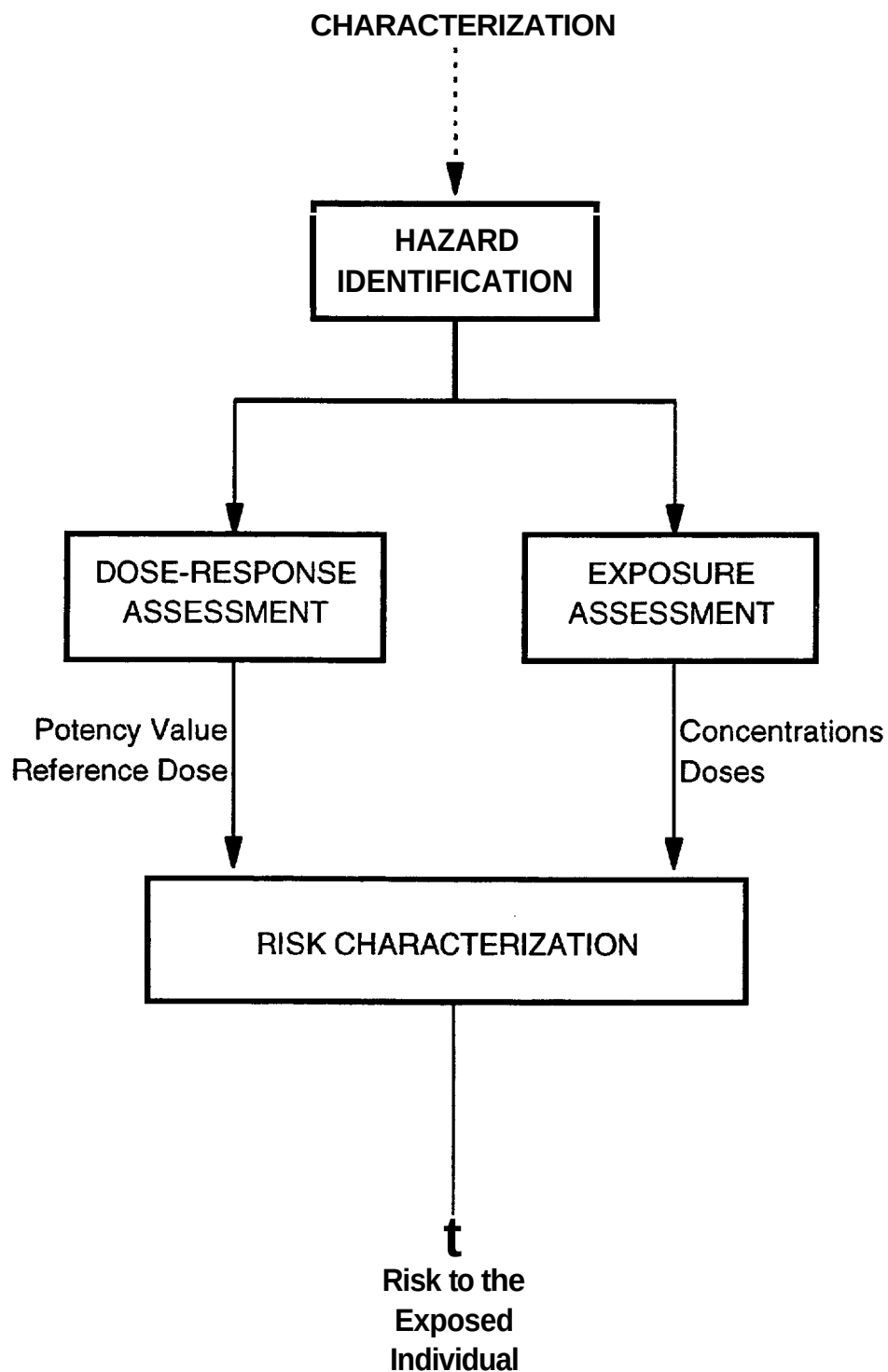


Figure 1-1. Schematic of the Risk Assessment Process.

In the hazard identification step, the chemicals of concern and the hazard (carcinogenic or other adverse health effects) associated with exposure to these chemicals are determined. This step necessitates collection of site-specific information to characterize the site in terms of source-, media-, chemical-, and receptor-specific characteristics. Potential receptors of concern and exposure routes are also identified in this step.

The objective of the exposure assessment step is to estimate intake by the receptor(s) identified in the previous step. This is a two-step process. First, the concentrations in the contact media (soil, air, groundwater), termed "receptor point concentrations" are estimated, and then the intake (or dose) is calculated for the receptor. Receptor point concentrations are actual or projected concentrations in site media to which a receptor (human) may potentially be exposed for particular pathways. For example, a receptor point concentration for groundwater could be the contaminant concentration projected to occur at a hypothetical or actual well location some distance from a source. Estimation of the receptor point concentrations is a key component of the exposure assessment step. This estimation often involves the use of contaminant fate and transport models and historical site data to simulate the movement of the chemicals of concern from the source to the receptor point. Contaminant fate and transport modeling should be calibrated with site-specific data. Once receptor point concentrations have been estimated, contaminant intake by the receptors is estimated.

Toxic effects of the chemical are identified and quantified in the dose-response assessment step. For carcinogenic chemicals, toxicity is quantified by estimating the chemical-specific potency value (also called slope factor). For non-carcinogenic chemicals, toxicity is quantified as the chronic reference dose, an estimate of the threshold daily level of exposure to the human population, including sensitive subpopulations, that may cause a deleterious health effect.

Finally, the risk characterization step combines the results of exposure and dose-response assessments to evaluate site-specific risk to the exposed populations. Each of these steps is described in detail in the subsequent sections of this manual.

The risk assessment process described above is very general in its application. Most state and federal regulations and associated guidance documents require risk assessments be conducted according to this process. However, there are many differences in the actual details of any given risk assessment. For example, risk may be based on arithmetic or geometric mean concentrations in the contact media. Similarly, there are a number of ways in which chemical concentrations reported as below the analytical detection limit may be treated. Additional variations exist in the estimation of the frequency and magnitude of contact media uptake. Details of these variations are not discussed in this manual. The manual and software generally follow the guidance presented in EPA (1989a).

1.3 OVERVIEW OF THE DECISION SUPPORT SYSTEM

This DSS consists of four modules coupled together into an integrated, user-friendly exposure/risk assessment framework. These modules are Development of Risk Scenario, Receptor Point Concentrations, Chemical Intake and Risk Calculation, and Risk Presentation.

The Development of Risk Scenario module allows the user to develop a conceptual model of the site for the purposes of risk assessment. In this conceptual model, the user identifies chemicals of concern, relevant uptake routes, and the specific models to estimate receptor point concentrations. Prior to running this module, an adequate site assessment should have been conducted, which helps ensure that the location is sufficiently well understood so that appropriate data are used in the DSS. This step corresponds to the last part of a "Hazard Identification" step shown in Figure 1-1.

The Receptor Point Concentrations module includes models to simulate contaminant fate and transport from source to receptor, thereby estimating receptor point concentrations. These models include atmospheric emission and dispersion models, and unsaturated and saturated zone contaminant transport models. It is important that the models used be calibrated with field data to help prevent inaccurate estimates. Alternatively, the user may enter directly into this module site-specific measured receptor point concentrations or those estimated by models

external to the DSS. The Receptor Point Concentrations module corresponds to the first part of the "Exposure Assessment" step shown in Figure 1-1.

The Chemical Intake and Risk Calculation module uses the computed or user-entered receptor point concentrations or user-entered concentrations to estimate chemical intake by the human receptor for several different exposure routes. These routes include ingestion of contaminated water and soil, inhalation of air containing volatile contaminants, and dermal contact with contaminated soil and water. This module also estimates the carcinogenic risk and non-carcinogenic effect (hazard index) due to these exposures. The Chemical Intake and Risk Calculation module corresponds to the second part of the "Exposure Assessment" step shown in Figure 1-1. Usually, toxicity parameters are obtained from EPA databases or other sources of published values. These toxicity parameters are specified in this module. Obtaining (or deriving) the toxicity parameters for the chemicals of concern corresponds to the "Dose-Response Assessment" step shown in Figure 1-1.

Finally, the Risk Presentation module uses EXCEL[®] to present the estimated chemical intake, carcinogenic risk, and hazard index. Several graphical and tabular options for presentation of results are available to the user. The results shown in the Risk Presentation module correspond to the "Risk Characterization" step shown in Figure 1-1.

An important aspect of this DSS is not only its ability to estimate the risk but also to evaluate the uncertainty in the risk estimates due to uncertainty in, and variability of, the input parameters. This uncertainty is quantified by using the Monte Carlo simulation technique. Monte Carlo simulation generates a probability distribution of the risk. From this distribution, the range as well as the most likely value (i.e., the 50th percentile) and the upper bound (i.e., the 95th percentile) can be estimated.

1.4 REPORT ORGANIZATION

This report includes the technical details and other information necessary to understand API DSS Version 2.0. Section 2.0 describes the overall structure of the decision framework and the hardware and software requirements of the system.

Section 3.0 includes instructions for using the DSS. Section 4.0 describes the details of the Development of Risk Scenario module and the development of a conceptual model of the site for the purposes of the risk assessment. Section 5.0 presents instructions on how to use the Receptor Point Concentration module. (The appendices of this manual contain detailed descriptions of the fate and transport models.) Section 6.0 describes the Chemical Intake and Risk Calculation module and includes the mathematical relationships used to estimate the intake, risk, and hazard index for each exposure route. Section 7.0 describes the Risk Presentation module and the available output formats. Sections 8.0 and 9.0 describe the DSS Monte Carlo uncertainty analysis procedures and the contents of the DSS databases, respectively.

This report also includes several appendices that provide the details of each fate and transport model included in the DSS, limited guidance for estimating values of selected input parameters, the probability distributions that can be used to describe the uncertainty and variability in the input variables, and the cumulative probability distributions based on data presented in the Exposure Factors Handbook (USEPA, 1989b).

2.0 STRUCTURE OF THE DECISION SUPPORT SYSTEM

In the following sections the various components of the DSS, as well as overall system requirements, software architecture, and flow of information will be described.

2.1 SYSTEM REQUIREMENTS

The DSS is a **Windows®**-based software and will run under Windows®.1 or Windows^m 95 and 98 with the following minimum hardware and software requirements.

2.1.1 Minimum Hardware Requirements

The API DSS requires the following configuration:

- An Intel® **486** or any 100%-compatible machine running at **25MHz** or faster
- At least 8 megabytes of RAM
- Math coprocessor
- At least 8 megabytes of free space on the hard-disk drive

2.1.2 Software Requirements

The API DSS requires the following software:

- Microsoft Windows^e **3.1, 95, 98**, or NT
- Microsoft EXCEL^m **5.0** (or higher version) for **Windows®**

2.2 DSS ORGANIZATION

The DSS consists of four modules as shown in Figure 2-1. These are the (i) Development of Risk Scenario, (ii) Receptor Point Concentrations, (iii) Chemical

Intake and Risk Calculation, and (iv) Risk Presentation modules. Each of these modules accesses databases and runs different computational codes as needed. The options available in, and data generated by, each module are shown in Figure 2-1. The structures of the databases are described in Sections 6 and 9. FORTRAN computational codes are run in both the Receptor Point Concentrations and the Chemical Intake and Risk Calculation modules as discussed in Section 2.3. DSS results are presented using EXCEL[®] macros. These macros are discussed in Section 2.4.

2.3 FORTRAN CODES

FORTRAN codes are used in the DSS for estimating receptor point concentrations and for calculating dose and risk. Fate and transport codes used to estimate receptor point concentrations are run in a deterministic mode. The risk calculation code may be run either deterministically or in a Monte Carlo mode. The risk calculation code is linked to a Monte Carlo software code so that uncertainty analyses can be performed easily. Details of the Monte Carlo code are discussed in Section 8.0.

The DSS collects all the information necessary to run each FORTRAN code, generates an input file on the hard drive, then runs the code. A new window appears and the FORTRAN code runs in this window, so the user can track the progress of the simulation. Successful completion of the FORTRAN run results in a message on the screen "Error Code = 0", see Figure 2-2. The user is also prompted to close the window and return to the DSS (select "Yes"). If the user wants to scroll through the screen output generated by the code, he or she can leave the window open (select "No") and look at the output. Before returning to the DSS, the user must close the FORTRAN window (select "File" from the menu bar, then "Eat", see also Section 3.3.6).

1. DEVELOPMENT OF RISK SCENARIO MODULE

Purpose: To **define** the risk scenario being evaluated.

User Identifies:

Chemicals of concern

Exposure routes

Method(s) of estimating Receptor Point Concentrations

Module Output:

Once the above information is specified a summary of data required to perform analysis based on selected options can be generated from the main screen.

2. RECEPTOR POINT CONCENTRATIONS MODULE

Purpose: To **enter** or **estimate** receptor point concentrations.

User Input: Receptor point concentrations **and/or** data for the fate and transport models.

The following transport models are available to estimate receptor point concentrations in the contact media:

Contact Media

Groundwater:

Model

SESOIL linked with AT123D

VADSAT

Jury linked with AT123D

AT123D

Air:

Emission

Jury

Thibodeaux-Hwang

Farmers

VADSAT

Box

Gaussian

Cowherd

Module Output:

EXCEL* tables and charts.

FORTTRAN output files summarizing all inputs and results.

Figure 2-1. Overview of the DSS.

3. CHEMICAL INTAKE AND RISK CALCULATION MODULE

Purpose: To **calculate** chemical dose and risk.

User inputs:

Exposure data
Toxicity data

Output:

EXCEL charts and tables containing the risk assessment results.
FORTRAN output file (INTAKE-OUT) summarizing all inputs and results.

4. RISK PRESENTATION MODULE (can also be accessed from the Chemical Intake and Risk Calculation module)

Purpose: To **present** results from the risk assessment.

No user input.

This module uses the EXCEL[®] spreadsheet to present report ready tables and charts of dose, risk and hazard index.

Module Output:

User can print or save the charts and tables and load them into other word processing programs.

Figure 2-1. Overview of the DSS (concluded).

2.4 EXCEL[®] MACROS FOR PRESENTATION OF RESULTS

The EXCEL[®] spreadsheet is used by the DSS to present results of the analysis. EXCEL[®] macros are used to provide the specialized functions for the DSS. These macros bring up a new menu item within EXCEL[®] allowing the user to select various tables and charts of results for both receptor point concentrations (accessed in the Fate and Transport module) and risk and hazard indices (the Risk Presentation module).

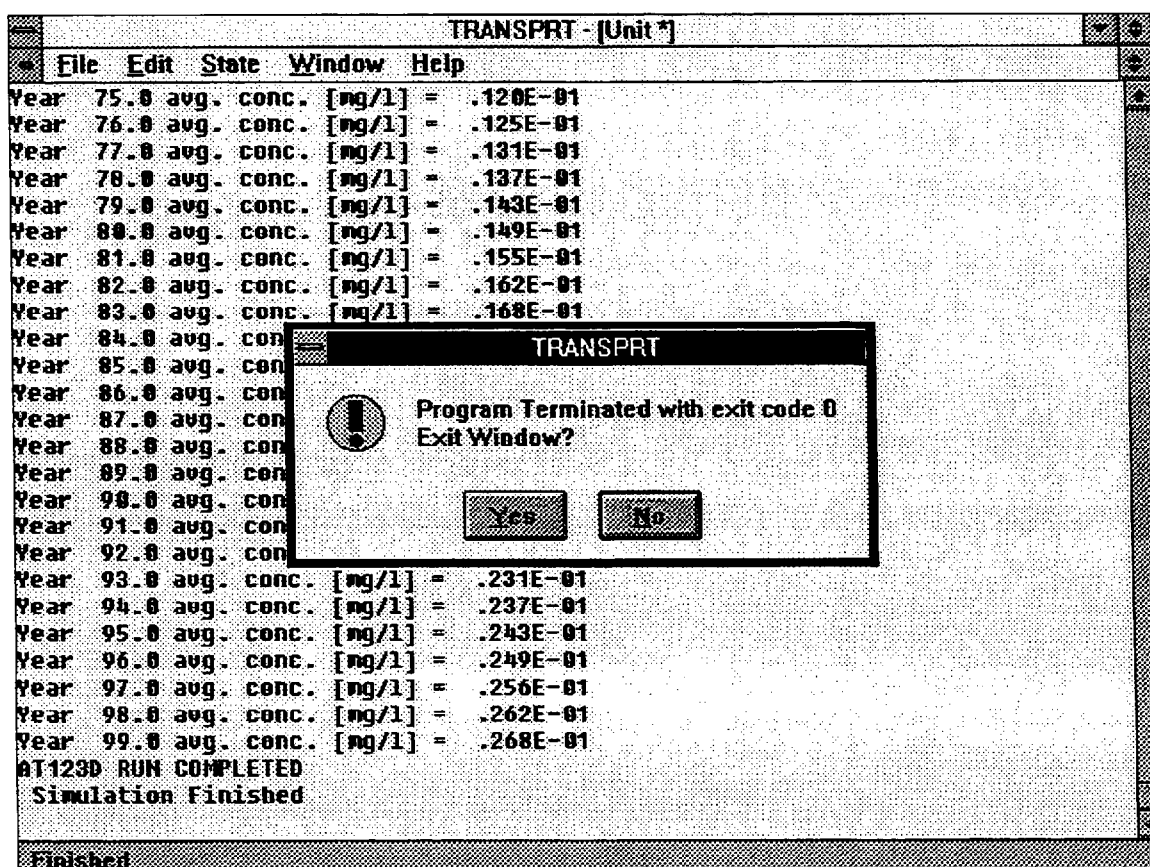


Figure 2-2. FORTRAN Code Completion.

The EXCEL[®] spreadsheet is accessed directly by the DSS; the user does not have to exit the DSS to run EXCEL[®]. After a FORTRAN run has been completed successfully, the EXCEL[®] button on the DSS screen becomes available. When selected with the mouse, the EXCEL[®] spreadsheet comes up automatically.

Once in **EXCEL**[®] there is a new menu option called "DSS" on the menu bar at the top of the **EXCEL**[®] window. When chosen, the "DSS" menu option brings up more menus from which the user can choose specific tables and graphs.

The **EXCEL**[®] macros create plots and tables of model output as shown in Section 7.0; however, users are free to modify the plots (using the standard **EXCEL**[®] commands) if they prefer a different font or type of plot. Also, the user can modify the format of the tables if desired (again, using standard **EXCEL**[®] commands). The tables and charts can be printed directly from **EXCEL**[®] just as from any other **EXCEL**[®] spreadsheet.

3.0

INSTRUCTIONS FOR USING THE DECISION SUPPORT SYSTEM

The DSS is designed to be user friendly with online help. This section will describe the installation procedures, as well as describe some of the system limitations.

3.1 INSTALLATION PROCEDURE

For Windows^m 3.1:

Step 1 Insert Distribution Disk #1 in drive A or B.

Step 2 Select "File" from the Program Manager menu and "Run" from the pull-down menu. Enter the following command in the dialog box:

a:\install.exe

Select OK on the Run dialog box.

Step 3 Follow the instructions in the installation package.

For Windows^B 95.98. and Windows^m NT:

Step 1 Insert Distribution Disk #1 in drive A or B.

Step 2 Select the "Start" button and then "Run..." from the pop-up menu. Enter the following command in the "Open" dialog box:

a:\install.exe

Select OK.

Step 3 Follow the instructions in the installation package.

3.2 STARTING A SESSION

To start the DSS, double-click on the API DSS icon in your Windows[®] desktop. The main menu of the DSS is shown in Figure 3-1. This screen has five buttons in the center. The top four correspond to the four modules of the API DSS. Only the first button is enabled, indicating that this step must be performed first. When the first step has been performed the other buttons will become available as appropriate.

At the bottom of the screen are four buttons: Quit, Load a Session, Help, and Save a Session. The Help button, when chosen with the mouse, brings up the help system for the DSS. The help system provides help for the current screen; the user is free to view the help index and display help for any listed topic. When Quit is chosen, the user will be prompted to save the session before exiting. When the "Load a Session" button is chosen, the user will be prompted to load a previously saved file. The "Save a Session" button allows the user to save data entered in the current session without having to leave the DSS.

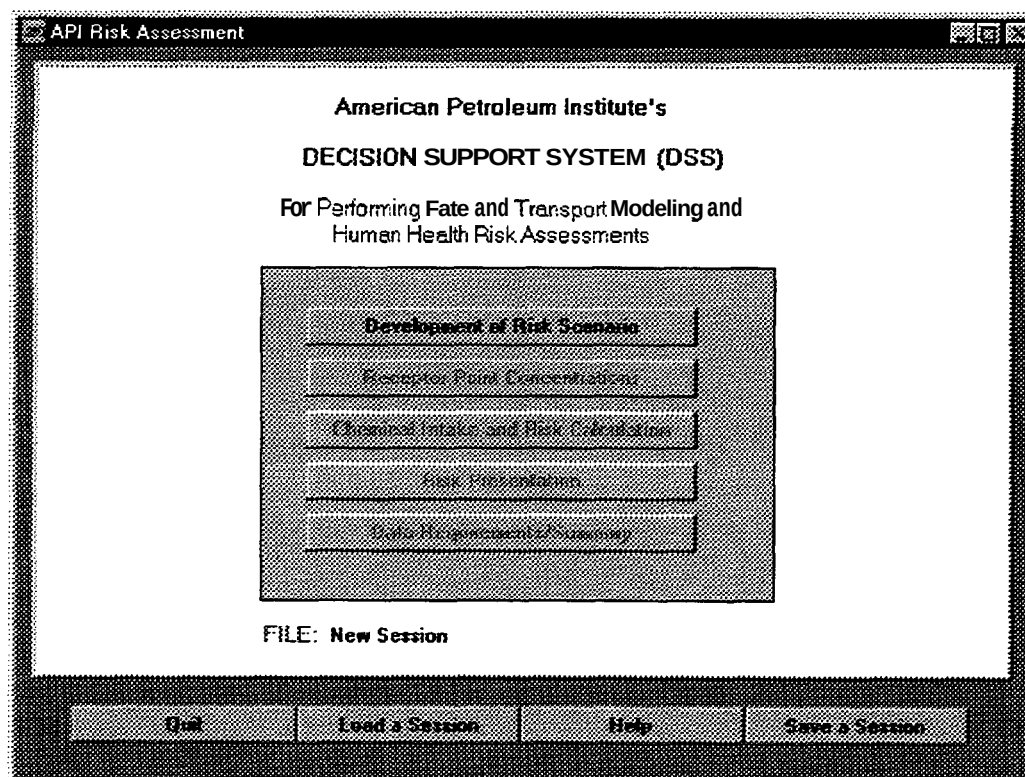


Figure 3-1. The Main Menu.

3.3 HOW TO USE API DSS

This section describes the screen formats **observed** when using the DSS and the types of information available from the different modules. It is recommended that the user run the DSS while reading this section.

3.3.1 Choose Options With a Single-Click

The only time the user should double-click the mouse is to start the DSS from the **Windows®** desktop or to close a window. Once in the DSS, the user chooses options such as buttons or hypertext by **single-clicking** with the mouse button.

3.3.2 Hypertext

Hypertext is special text (highlighted in green) which can be selected as a topic by clicking with the mouse. Selecting hypertext usually displays additional information on the word or phrase that was highlighted. Hypertext in the DSS is highlighted in green. The mouse cursor changes to a hand when it is over Hypertext.

3.3.3 Screen Layout in the DSS

The basic format of the DSS screens consists of a maximized window with a title bar and a control menu (the **box** at the left side of the title bar, refer to Figure 3-1). The title bar shows the application name "API Risk Assessment." The control menu allows the window to be minimized or moved. The control menu allows the user to switch to other **Windows®** programs if desired. Another way to minimize the window is to click on the down arrow on the right side of the title bar.

3.3.4 Buttons, Drop-Down Lists, and Edit Boxes

Within the modules, the user should click on the button corresponding to the desired step. After entering all the appropriate information for that step, the user is returned to the module window and the box next to the selected button will be checked.

Occasionally, some of the buttons will be disabled (shaded) indicating that other information is needed before that step can be performed. For example, in the **AT123D** initial input screen the aquifer data cannot be entered until the **AT123D** model control parameters are chosen. Once these control parameters have been entered the aquifer data buttons will become available.

Edit boxes are used wherever the user may want to change the default values (e.g., model parameters, title boxes). These boxes may be edited by clicking on the edit box with the mouse and typing a new value.

A drop-down list (i.e., a box with a down arrow on the right) is used to select a value from a list of options. When the down arrow is selected, a list will appear and the user can select any item on the list. When an item from the list is selected, the **drop-down** list will close and the new default will appear in the box. This type of drop-down list is used to choose among the various distribution types in the Monte Carlo mode.

3.3.5 HELP System

The DSS has on-line help that is available from every screen. This feature can be activated by choosing the HELP button (located at the bottom of the screen) with the mouse. This displays the Help Window that has (i) topic specific information and (ii) a menu bar at the top with six buttons (Contents, Search, Back, Copy, Print and Quit) that perform the following functions:

- Contents: Displays the list of contents (modules and databases) of the DSS.
- Search: Displays a list of all the HELP topics (in alphabetical order) included in the DSS. The user may choose any topic to view information on that topic.
- Back: Displays the previous topic.
- Copy: Copies the contents of the HELP window into the Windows@ Clipboard. The text can then be transferred to a word processing file.

- Print: Sends the HELP text directly to the printer
- Quit: Closes the window and returns the user to the **DSS**.

Note, some of the text displayed in the HELP window is highlighted in green. This is HYPERTEXT and can be selected by the user (by clicking) to view additional information on the topic.

3.3.6 Running FORTRAN Codes

The computational elements of the **DSS** are **written** in FORTRAN and include (i) the models in the Receptor Point Concentrations Module and, (ii) the algorithms to compute dose, carcinogenic risk and the hazard index in the Chemical Intake and Risk Calculation Module. The FORTRAN codes are executed by selecting the "Run" button. This button is not available until all the data required to run the FORTRAN codes have been entered. Quantitative data can be entered in either floating point, integer, or exponential form. The number of significant digits is left to the user's discretion. The interface performs limited range checking but users are cautioned to enter the appropriate value and not rely solely on the interface to check the appropriateness of a data value.

The **DSS** runs each FORTRAN code in a window that displays the code's output as it is generated. The sole objective of the screen output is to monitor the progress of the computations (e.g., the number of Monte Carlo runs completed). At the completion of the run a message is displayed on the screen which shows (i) an error code of either 1 or 0 and (ii) a query prompting the user to exit the FORTRAN window (Figure 2-2). An error code of 0 indicates successful completion of the FORTRAN code. An error code of 1 indicates an unsuccessful completion - probably due to an error in the data entered. **In either case (an error code of 0 or 1) the user must exit the FORTRAN window before proceeding further.**

An "MSLANGLOAD (Microsoft Language Loader) error may occur if too many Windows^B applications are open or the computer does not have enough memory (RAM). If an MSLANGLOAD error occurs, the user should make sure that **all** other Windows^B applications are closed (e.g., EXCEL^B, DOS Shell, File Manager).

After the run has been successfully completed and the FORTRAN window has been closed, the **DSS** allows the user to select one of two options: (i) "View Charts and Tables in EXCEL," or (ii) "View FORTRAN Results." EXCEL^B outputs are discussed in Section 3.3.7 below. For SESOIL, AT123D, and Jury's model, these FORTRAN output files are similar to the output files a user would obtain by running these models outside the **DSS**. The FORTRAN output files may be printed from the interface.

3.3.7 Using EXCEL[®] with DSS

After running the FORTRAN code, the user can review the results in EXCEL[®] provided the directory containing EXCEL[®] has been added to the DOS path specified in the AUTOEXEC.BAT file (see Section 3.1). When running EXCEL[®] the user can view tables and charts showing the results of the analysis by choosing the "DSS option that has been added to the standard EXCEL[®] menu bar. These charts and tables can be printed or saved by using the "print" or "save" option respectively under the "file" menu. The tables contain the name of the analysis entered by the user before running the FORTRAN codes.

To exit EXCEL^B, use the "Return to DSS" option under the DSS menu item.

3.4 MONTE CARLO AND DETERMINISTIC MODES

The user can choose to run the risk calculation FORTRAN code in either a deterministic mode or a Monte Carlo mode. The default option is the deterministic mode, as indicated by the solid bullet in the first screen of the Chemical Intake and Risk Calculation module and each fate and transport model's main screen. To choose Monte Carlo mode, the user may click on the words "Monte Carlo." A new edit box will appear so the user can enter the number of Monte Carlo runs desired. The maximum number of runs is 10,000.

Under the Monte Carlo option, the format of the user input screens is altered. Whereas the deterministic input screens have only one edit box for each parameter, the Monte Carlo input screens allow the user to choose a distribution from a

drop-down list and then enter the statistical parameters needed to describe the distribution for each parameter. Available statistical distributions are: constant, normal, log-normal, exponential, uniform, and triangular. The statistical parameters that describe the distribution are mean, mode (for triangular distributions), standard deviation, minimum, and maximum. Additional details are included in Section 8.0 and Appendix K.

3.5 PRINTING

There are several places in the DSS where the user can print information, assuming that Windows@ has been configured to print. (If Windows® has not been configured to print, the user should follow the instructions in the Windows® manual and set up the appropriate printer.) The main screen of the API DSS has an option to print a summary of the data requirements for a given analysis. This summary is available from a button on the main module screen.

The tables and charts presented in EXCEL@ can also be printed. These are designed to be report-ready; the user can easily print them directly from EXCEL@'. Users experienced with EXCEL® may wish to reformat the tables and charts. Again, the charts can be saved as text files and brought into a word processing program.

The FORTRAN output files can also be printed. These output files ("*.out") are neither formatted nor report-ready; they are merely designed to provide summary statistics to the experienced user. After running any FORTRAN code, the user has the option to view a summary of the FORTRAN output. These files can be opened with a word processor (such as Microsoft Word®, or Write®) and reformatted.

3.5.1 Performing a Screen Dump to the Windows@Clipboard

The following steps describe how to perform a screen dump from the screen to the Windows@Clipboard.

Make sure the information you want to copy is on the screen. Press PRINT SCREEN. The contents of the screen are copied onto the Clipboard. If the above

procedure does not copy the screen onto the Clipboard, you may not have an enhanced keyboard. Try pressing **ALT+PRINT SCREEN** or **SHIFT+PRINT SCREEN** to copy the screen.

Choose the Clipboard Viewer icon in the Windows Main group to view the contents of the Clipboard. Switch to the destination application, i.e., the application from which you want to print (such as MS Word®, EXCEL® or Paintbrush®). Place the insertion point where you want the information from the Clipboard to appear. From the application's Control menu, choose Edit. From the Edit menu, choose Paste. The screen can now be printed from the application.

3.6 QUITTING AND SAVING USER PREFERENCES

Whenever a user quits a session in the DSS the user is prompted to save choices and results. Similarly, the data can also be saved without exiting the DSS by choosing the "Save a Session" button on the main screen. The information is saved in a user-specified file as compiled code (not editable). When a new session is started, the user has the option to load any of the previously saved files. Information from this file will appear as defaults for the current analysis.

3.7 LOADING A SAVED FILE

After a session has been saved (Section 3.6) it can be reloaded at a later time. This is accomplished by choosing the "Load a Session" button from the main menu (Figure 3-1). Clicking on the "Load a Session" button brings up a file selection window showing the files with the extension *.sav. If the saved file has a different extension the user can find the file by entering "*.*)" in the "File Name:" edit box. If the saved file is in another directory or drive the user can change directories by choosing the appropriate directory from the boxes in the window.

The saved file contains all the data entered in the session and the FORTRAN code results if a successful run was made. To transfer the saved file to another directory (or computer) just copy the saved file to the new directory (or computer).

3.8 SYSTEM LIMITATIONS

DSS limitations include:

- The maximum number of chemicals for a DSS session is limited to twenty.
- The DSS can only consider one receptor at a time. This limitation was imposed to simplify system output and its interpretation. If a user wants to analyze the risk posed to two different receptors, he or she may run the DSS twice. Default parameter values from the first analysis can be saved and then retrieved for the second analysis.
- The DSS includes six routes of exposure as discussed in Section 6.0. Other exposure routes such as the ingestion of produce grown in contaminated soil or the inhalation of indoor air in confined spaces (such as basements), are not addressed. Depending on the site-specific conditions, these routes of exposure may be significant.

Other assumptions and limitations include:

- The EPA Uptake Biokinetic model for lead is not included in the software. If lead is added to the DSS database, it will be treated in the same manner as other chemicals requiring a slope factor or reference dose.
- Risks are additive; chronic effects are additive.
- Risks are carcinogenic only. Teratogenicity, mutagenicity, etc., are not considered.
- Chronic toxicities are not specified by toxic effect or affected organ.
- Fate and transport models may assume steady-state and compositional equilibrium between phases at all times.

- Risk is to a maximally exposed individual. Population risks are not addressed.
- Subchronic risks are not addressed by the DSS. The database does not contain toxicity values for subchronic exposures (less than two years).
- **Risks/chronic** effects to children can be calculated by assuming that a child is a "small adult." It is assumed that potency factors, **RfDs**, apply to children as well as adults.

DEVELOPMENT OF RISK SCENARIO MODULE

4.1 OVERVIEW OF THE MODULE

An important first step in conducting a risk assessment is to develop a conceptual model of the site. Key elements of the conceptual model include identification of the contaminated media, the chemicals of concern, the types and locations of receptors, the relevant routes of exposure, and the manner in which the receptor point concentrations for each chemical are to be estimated. The Development of Risk Scenario module allows the user to define a conceptual model for the site-specific risk assessment by specifying three types of information. These are categorized as:

- i) chemicals of concern,
- ii) routes of concern, and
- iii) method for estimating receptor point concentrations.

Figure 4-1 shows the "Development of Risk Scenario" input screen. The first button is where the chemicals of concern are chosen. The second button is where the routes of exposure and the method for estimating receptor point concentrations are identified.

4.2 CHEMICALS OF CONCERN

Figure 4-2 shows the Chemicals of Concern screen. Chemicals of concern are selected from this list by clicking on the chemical(s) with the mouse and then choosing "Add→." A selected chemical may be deselected by clicking on it and selecting "←Remove." Version 2.0 of the DSS allows the user to select up to 20 chemicals of concern from a total of 48 chemicals included in the database. Use the up and down arrows to scroll through the chemicals listed in the database. New chemicals may be added to the DSS by choosing "Add Chemical to Database."

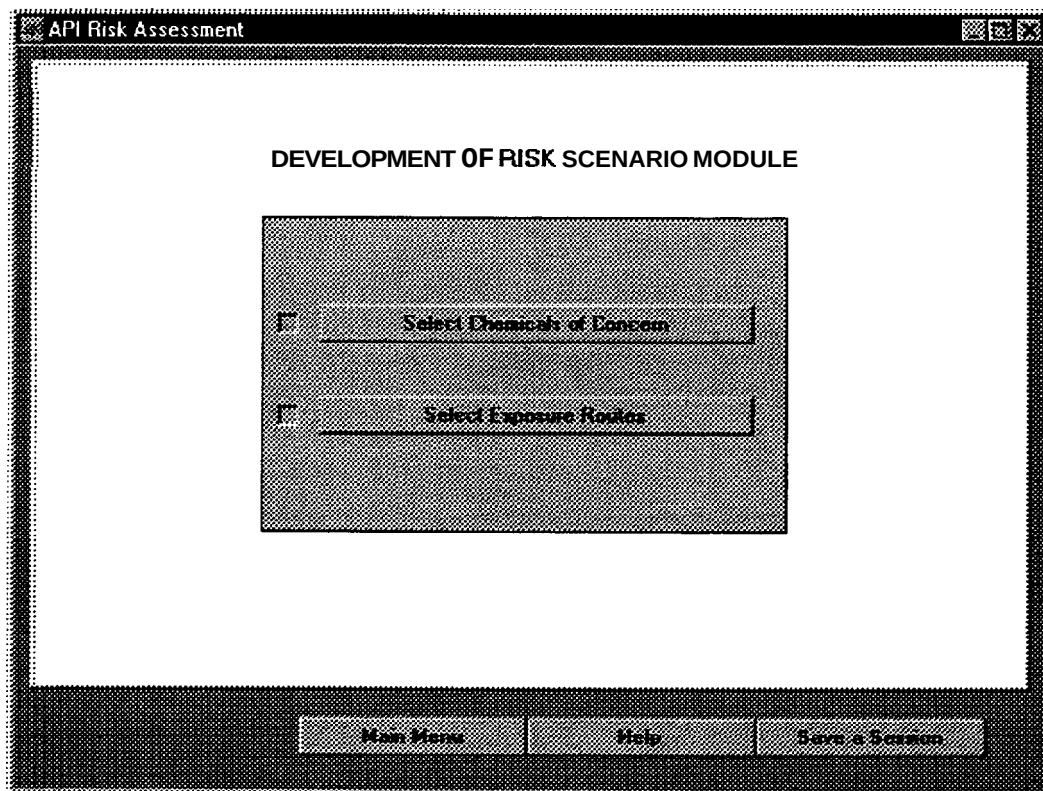


Figure 4-1. Development of Risk Scenario Screen.

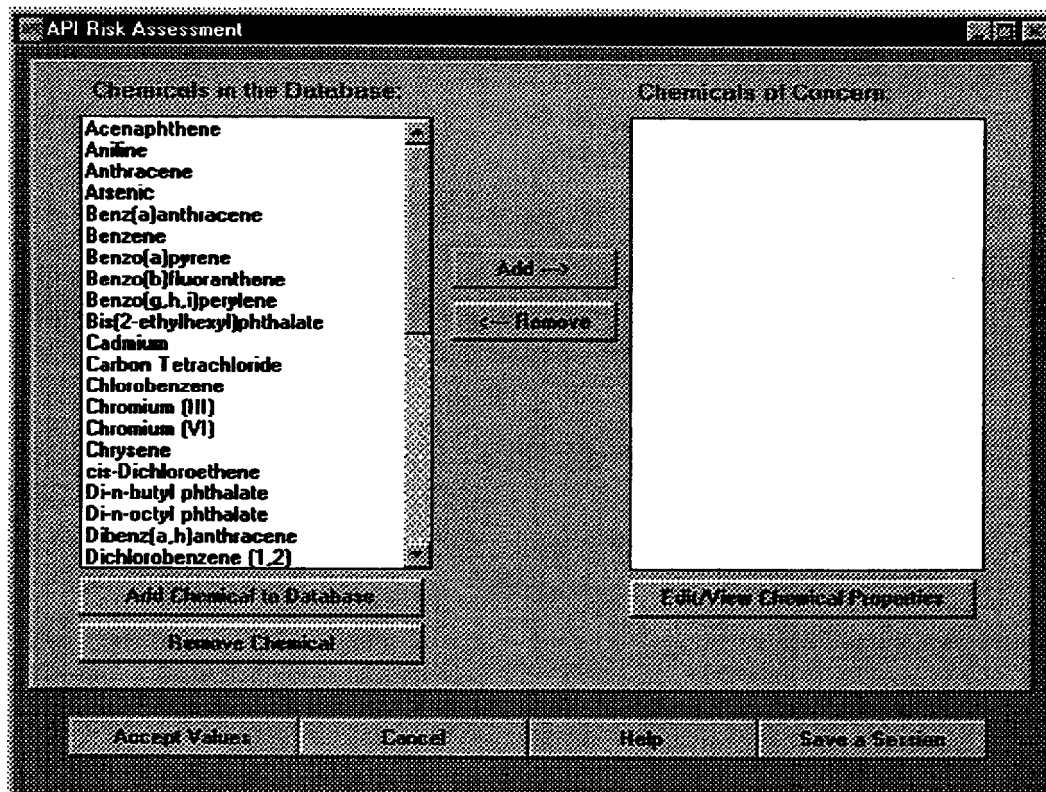


Figure 4-2. Selecting Chemicals of Concern.

The process for selecting chemicals of concern is described in the EPA Risk Assessment Guidance for Superfund manual (RAGS, EPA 1989a). Section 5.8 of the RAGS guidance lists the criteria for identifying chemicals of **potential** concern using site-specific information. Briefly, the initial chemical list should include chemicals that were:

- 1) positively detected in at least one sample;
- 2) detected at levels significantly elevated above levels of the same chemicals detected in associated blank samples;
- 3) detected at levels significantly elevated above naturally occurring background levels;
- 4) only tentatively identified but may be associated with the site historically; or
- 5) transformation (daughter) products of chemicals demonstrated to be present.

This initial list can be slimmed down using **toxicity/concentration** screens, etc. See the RAGS guidance for more information.

4.2.1 Edit/View Chemical Properties

By selecting this button, the user may view or change the values for the chemical properties for each chemical in the API DSS database. Please note, if the values are changed in this location they will be permanently changed in the database. If the values were changed mistakenly, the user either can change them back (using the values presented in the manual, Table 9-1) or reload the API DSS from the installation disks. This process will just **overwrite** the files used to run the program and will not overwrite any saved session files.

4.3 ROUTES OF CONCERN

From the Development of Risk Scenario screen, the user must also choose the exposure routes of concern. There are six routes available in the DSS:

- 1) Ingestion of Drinking Water
- 2) Dermal Absorption while Bathing
- 3) Inhalation while Showering
- 4) Inhalation of Soil Emissions
- 5) Dermal Contact with Soil
- 6) Ingestion of Soil

API Risk Assessment

Select Routes of Concern and Concentrations:

☒ Drinking Water
☒ Dermal Intake During Shower
☒ Inhalation During Shower
☒ Inhalation of Soil Emissions
☒ Dermal Contact with Soil
☒ Soil Ingestion

Groundwater Concentration:

☐ User specified concentrations
☒ Use model to estimate concentrations

☐ AT123D
☐ SESOIL followed by AT123D
☐ SESOIL with Mixing Zone
☐ Jury followed by AT123D
☒ VADSAT

Air Concentration:

☐ User specified concentrations
☒ Use model to estimate concentrations

Volatile Emissions Model:

☐ Jury
☐ Thibodeaux-Hwang
☐ Farmers
☐ SESOIL
☒ VADSAT
☐ User specified emissions

Dispersion Model:

☒ Box
☐ Gaussian

Calculate Particulate Emissions:

☐ Yes ☒ No

Soil Concentration:

☒ User specified concentrations

Accept Values Cancel Help Save a Session

Figure 4-3. Selecting Routes of Concern.

These routes are displayed on the top of the "Select Routes of Concern" screen (Figure 4-3). The user should select exposure routes based on the receptor **type** and expected location of the receptor. For example, if risks to an on-site resident are being estimated, then all the above routes may be of concern. On the other hand, if an on-site worker is being considered, the shower routes may **be** eliminated leaving inhalation of soil emissions, dermal contact with soil, soil ingestion, and ingestion of groundwater as routes of concern. Of course, if showers are available

to the workers at the site (and the showers use groundwater) then the shower routes should be considered for a worker scenario.

Table 4-1 lists suggested exposure routes for different combinations of receptor type and the contaminated media. As an example, if soil is contaminated at a given site and the receptor is an off-site resident, ingestion of contaminated soil and dermal absorption of chemicals due to contact with soil are not considered viable routes of concern. However, chemicals may leach from the soil into groundwater so the groundwater routes are potential routes of concern. Similarly, chemicals may volatilize from the soil into the air, making inhalation of soil emissions a pathway of concern.

When a route of concern is selected from the interface, the associated media concentration box (below the Routes of Concern) becomes available. For example, when the user selects "Drinking Water" as a route of concern, the "Groundwater Concentration" group becomes available indicating that the user needs to **specify** the methodology for estimating receptor point concentrations. This process is explained in the following section.

4.4 RECEPTOR POINT CONCENTRATION ESTIMATION METHODOLOGY

Receptor point concentrations in the contact media are necessary variables for computing chemical intake. Depending on the routes of concern identified, receptor point concentrations may be required for air, groundwater, and soil. For example, if the only exposure routes to be analyzed are ingestion of soil and dermal absorption of chemicals due to contact with soil, the only receptor point concentrations required are the concentrations in soil.

In general, receptor point concentrations for each medium can be estimated by: (i) analysis of site-specific data, or (ii) application of fate and transport models. In the "Select Routes of Concern" screen (Figure 4-3), the user identifies the method to **be** used to estimate concentrations for each medium of concern (groundwater, soil, and/or air).

TABLE 4-1. Suggested Routes of Exposure for Selected Receptor Type and Contaminated Medium.

Receptor Type and Location	Contaminated Media	Possible Routes of Exposure					
		1	2	3	4	5	6
On-site Resident	Soil	•	•	•	•	•	•
	Groundwater	•	•	•	—	—	—
	Air	—	—	—	•	—	—
Off-site Resident	Soil	•	•	•	•	—	—
	Groundwater	•	•	•	—	—	—
	Air	—	—	—	•	—	—
On-site Worker	Soil	—	—	—	•	•	•
	Groundwater	•	—	—	—	—	—
	Air	—	—	—	•	—	—
Off-site Worker	Soil	—	—	—	•	—	—
	Groundwater	•	—	—	—	—	—
	Air	—	—	—	•	—	—
Visitor	Soil	—	—	—	•	•	•
	Groundwater	—	—	—	—	—	—
	Air	—	—	—	•	—	—

1. Ingestion of water
2. Dermal absorption while showering
3. Inhalation while showering
4. Inhalation of emissions from soil
5. Dermal contact with soil
6. Ingestion of soil

If the first option is selected (using site-specific data), the receptor point concentrations are entered by the user in the Receptor Point Concentrations module. If the second option is selected (using fate and transport models), the user must specify which **model(s)** will be used. The fate and transport models included in the DSS are described in Section 5.0 and Appendices A through H, and O. The available choices are shown in Figure 5-1. Receptor point **concentrations may** be user-entered for some media and calculated for others.

In some cases the fate and transport models are linked together. For instance, **SESOIL** (a vadose zone model) may be used to calculate contaminant mass loading to groundwater and volatile emission rates. Both of these outputs are used as inputs to other models. The loading to groundwater is used as an input to the saturated zone model, **AT123D**, and the volatile emission rates are used as input to an air dispersion model (either box or Gaussian) if the air pathway is being considered.

4.5 DATA REQUIREMENTS SUMMARY

The data required to estimate the risk at a site depend on the conceptual model developed. Thus, the necessary data depend on the type and location of the receptor, the contaminated media, the method of estimating receptor point concentrations, and the relevant routes of exposure. Based on the decisions made by the user, as discussed above, the DSS summarizes all the data that will be necessary to estimate the risk. This information is available from the "Data Requirements/Summary" button on the main API DSS screen (Figure 3-1).

An example of this summary is included in Table 4-2. Specific values for these parameters can be estimated based on a combination of site-specific field investigations, a literature search, professional judgment, or default values included in the DSS databases discussed in Section 9.0. It is recommended that while conducting a site assessment or risk assessment the user print this list and select values for each parameter before proceeding on to the site assessment or to the next module. Appendix J also includes a list of the input variables and guidance on estimating their values.

If the "Data Requirements/Summary" button is chosen after information has been entered in the DSS, the output will summarize the values entered.

Table 4-2. Printout of the Data Requirements/Summary Option.

API DSS Data Requirements Example 10/25/97 10:08

DEVELOPMENT OF RISK SCENARIO

The following chemicals were selected:

Benzene
Ethylbenzene

The following exposure routes were selected:

Drinking Water
Inhalation During Shower

RECEPTOR POINT CONCENTRATIONS

User-Specified Receptor Point Concentration Distributions

Groundwater Concentrations [mg/L]

Benzene	0.0
Ethylbenzene	0.0

INTAKE PARAMETERS

Analysis Type: —

Body Weight and Lifetime

Average Weight (kg)	—
Lifetime (yrs)	—

Drinking Water

Exposure Frequency [days/yr]	—
Exposure Duration [years]	—
Ingestion Rate [liters/day]	—

Drinking Water Chemical Specific Parameters

Benzene	
Bioavailability [fraction]	1
Ethylbenzene	
Bioavailability [fraction]	1