NATURAL ATTENUATION SOFTWARE (NAS)

User's Manual

Version 2

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by

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DISCLAIMER

NAS is made available on an as-is basis without guarantee or warranty of any kind, expressed or implied. The US Navy, USGS, Virginia Tech, any of the authors accept no liability resulting from the use of NAS or its supporting documentation. Implementation of NAS and interpretation of the predictions of the model are the sole responsibility of the user.

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Introduction

Purpose and Scope

Natural Attenuation Software (NAS) is a screening tool to estimate remediation timeframes for monitored natural attenuation (MNA) to lower groundwater contaminant concentrations to regulatory limits, and to assist in decision-making on the level of source zone treatment in conjunction with MNA using site-specific remediation objectives.

NAS is designed for application to ground-water systems consisting of porous, relatively homogeneous, saturated media such as sands and gravels, and assumes that groundwater flow is uniform and unidirectional. NAS consists of a combination of analytical and numerical solute transport models. Natural attenuation processes that NAS models include advection, dispersion, sorption, non-aqueous phase liquid (NAPL) dissolution, and biodegradation. NAS determines redox zonation, and estimates and applies varied biodegradation rates from one redox zone to the next. NAS models are implemented in three main interactive modules to provide estimates for:

1. **Required Source Reduction:** target source concentration required for a plume extent to contract to regulatory limits (i.e. **Distance of Stabilization (DOS)**),

2. **Time of Stabilization (TOS):** time required for a plume extent to contract to regulatory limits after source reduction.

3. **Time of Remediation (TOR):** time required for NAPL contaminants in the source area to attenuate to a predetermined target source concentration, and

With the successful development of the initial version of NAS and application of NAS to several contaminated sites, several critical needs had been identified. Software enhancements have been implemented to improve NAS and maximize its utility for site managers. Including general operational and functional revisions, NAS has expanded source contaminant specification options to include chlorinated ethanes, chlorinated methanes, and chlorinated benzenes, and to allow for the analysis of any other user-defined contaminants that may be subject to microbially-mediated transformations (e.g., heavy metals, radioisotopes, etc.). Included is the capability to model co-mingled plumes, with constituents from multiple contaminant categories. To enable comparison of remediation timeframe estimates between MNA and specific engineered remedial actions (ERAs), NAS was modified to incorporate an estimation technique for timeframes associated with pump-and-treat remediation technology for comparison to, or in conjunction with, MNA. NAS is now able to model sites with existing or proposed pumping wells, based on user-specified site hydrogeologic and source data. NAS also includes expanded analysis tools for improved performance assessment. Sustainability of natural attenuation processes over time may also be assessed. Users may analyze historically successive, site-measured, contaminant concentration and redox indicator data, to allow for comparisons of NAS-predicted versus observed trends, and to monitor changes in natural attenuation capacities and redox conditions over time.

Minimum Site Data Requirements

First, detailed site information about hydrogeology, redox conditions, and contaminant concentrations must be entered. Table 1 provides a summary of the basic site data required by NAS. NAS is primarily designed as a screening tool early in the remedial strategy selection process following completion of site investigation and characterization. If the data NAS requires is not available, then time of remediation estimates can not and should not be made. However, another use of NAS is to reveal site data deficiencies that can be addressed during the remedial strategy selection process and to develop monitoring strategies.

Table 1. Summary of Basic NAS Site Data Requirements

Hydrogeology	**Required**
Hydraulic conductivity	Best estimate, maximum, minimum values
Hydraulic gradient	Best estimate, maximum, minimum values
Weight percent organic carbon	Best estimate, maximum, minimum values
Total Porosity	Best estimate
Effective Porosity	Best estimate
Contaminant source width	Best estimate
Contaminant source length	Best estimate
Average saturated thickness impacted by contamination	Best estimate
Redox Indicators	
Concentration: Dissolved oxygen, Ferrous iron, Sulfate	Values from 1 or more wells along the solute plume centerline
(Optional) Concentration: Nitrate, Mn(II), Sulfide, Methane, Dissolved hydrogen	Values from 1 or more wells along the solute plume centerline
Contaminant	
Concentration: Contaminant	Values from 2 or more wells along the solute plume flow path

Overview of the NAS Interface

Figure 1 shows a flowchart describing how the NAS software can be used to address time of remediation questions. After data entry, NAS estimates site-specific ground-water flow rates, biodegradation rates, and sorption properties. Based on the range of estimates, NAS then produces either analytical or numerical solutions of the TOR equation. One option employs analytical solutions to determine the target reduction in the source area concentration to meet site-specific remediation goals. This approach and solution addresses plume concentration questions, such as what is the distance of stabilization for given source-area contaminant concentrations, and what is the time of stabilization if source-area concentrations are changed. For the distance of stabilization question, NAS calculates the allowable maximum source-area concentration, based on a regulatory maximum concentration level at a given point downgradient of the source. Then, NAS estimates how long it will take for the plume to reach the lower steady-state configuration once source-area concentrations have been lowered by engineering methods. Once both the distance of stabilization and the time of stabilization are

acceptable, based on site-specific regulatory criteria, MNA can become an integral component of site remediation.

The other option is a mass-based approach to determine the target reduction in the source area NAPL or residual mass to reduce the TOR based on site-specific remediation goals. To achieve this solution, NAS uses the SEAM3D code (Waddill and Widdowson, 1998) to solve the solute transport equation in conjunction with a groundwater flow code (MODFLOW). The solution provided by NAS is tailored to estimate the length of time required by a given NAPL mass to dissolve and lower contaminant concentrations at the source area below a given user-supplied threshold.

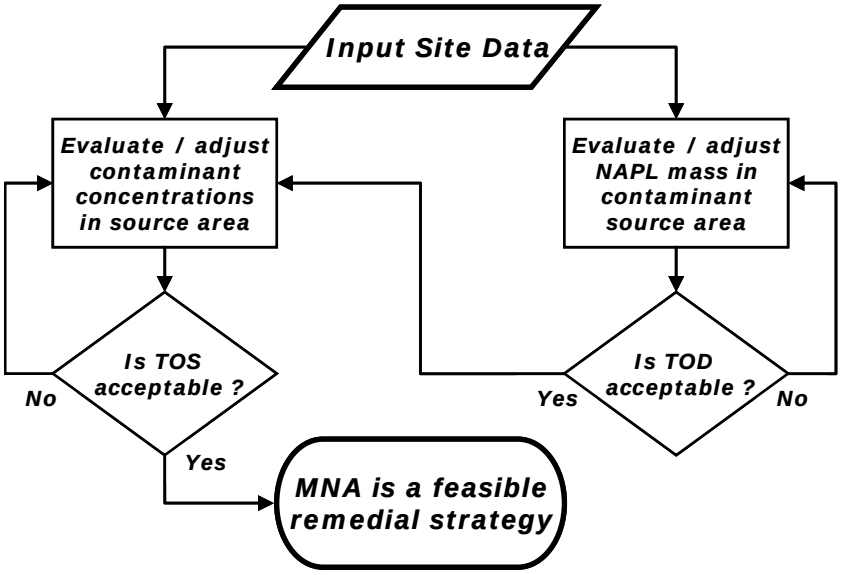


Figure 1. Flow Chart for the Application of NAS

Getting Started

Installation

To install NAS, click on the 'setup.exe' file and follow the instructions given. NAS has been designed to run in Windows operating systems.

Once NAS has been installed, the program may be started by clicking on the 'Start Button' (located at the lower left of the computer screen), then pointing to the 'Programs' folder, the 'Natural Attenuation Software' Subfolder, and finally the NAS program file. This procedure is shown in Figure 2 for a computer system running WindowsXP.

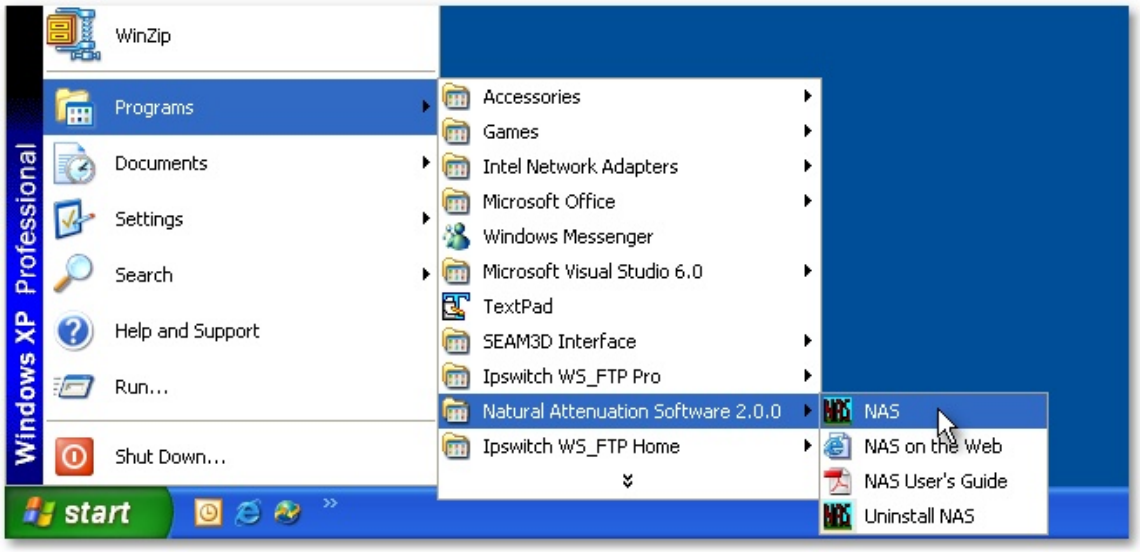


Figure 2. NAS from Start Button

Description of Program Directory

This section describes the Program Directory installed by the NAS setup program. Folders and files in the NAS Program Directory include:

Documentation: This directory stores the NAS User's Guide and any other Help documentation that may be distributed by a future version of NAS.

Tutorials: This directory stores the example NAS project files referenced by the NAS software. New tutorial files may be distributed to this folder by a future version of NAS.

Program Executables: 'NAS.exe' and 'NASShell.exe' are the main program executables and should not be removed from the directory.

Contaminant Database: 'NASDB.unf' and 'NASDBDefault.unf' are the NAS contaminant database files, in binary format, and should not be accessed/edited by the user. NAS can export/import this database to/from Excel format as will be discussed in a later section.

Program Support Files: 'LF90.EER', 'Olch2d-u.cnt', and 'Olch2d-u.hlp' are support files necessary for the proper functioning of NAS and should not be removed from the directory.

For proper functioning of NAS, all folders and files mentioned in this section should not be removed or changed. NOTE: It is also advised to not save NAS Project Files (*.nas) in the NAS Program Directory; save them in separately created directories instead.

Navigating the Main Menus

The first NAS screen shown after clicking on the NAS Program File is the main NAS working window with the Menu shown in Figure 3. The NAS Main Menu allows the user

to either perform various file operations or to enter one of the NAS program functions. Main Menu items include file operations (File), site data entry (Site), Source Concentration Reduction, and Distance/Time of Stabilization calculations (DOS/TOS), Time of Remediation calculations (TOR), tabular and graphical output of site data and results (Output), functions for managing program windows (Window), and NAS documentation and support (Help).

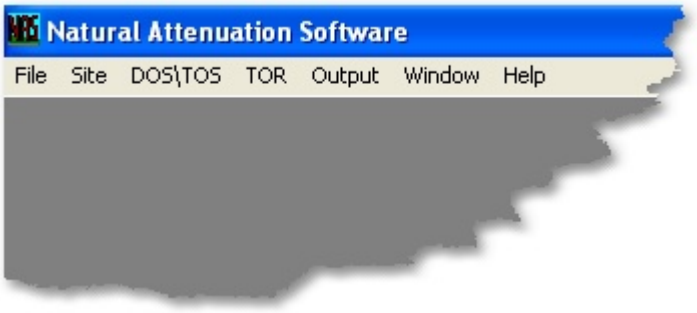


Figure 3. NAS Main Menus

File

The file operations available to NAS are shown in Figure 4.

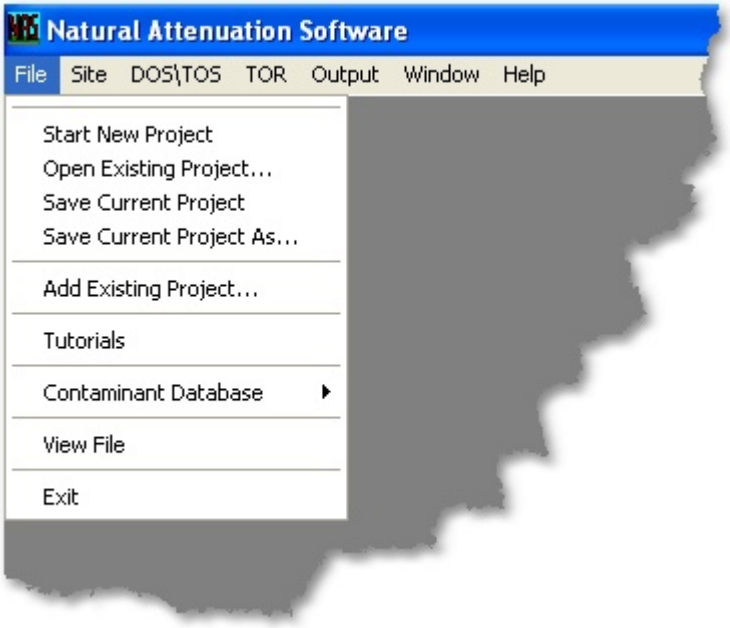


Figure 4. File Menu

Start New Project

To start a new project, open NAS and select the 'Start New Project' menu item. This action will take you to the 'General Tab' of the 'Site Data' Form. This form will be discussed in greater detail in a following section.

Open Existing Project

To open an existing project, open NAS and select the ‘Open Existing Project’ menu item. A standard Windows file open dialog box will appear, in which you may select the drive and directory where the NAS input file is listed. Note that the default naming convention for NAS project files is *.nas. The input format for this file is shown in Table 2 in Appendix A. Users familiar with the format may manually edit *.nas files. Any *.nas file may also be automatically opened in NAS by double-clicking the file in a Windows explorer window. This action will take you to the ‘General Tab’ of the ‘Site Data’ Form. This form will be discussed in greater detail in a following section.

Save Current Project (As)

To save a project currently loaded in NAS, select the ‘Save Current Project As’ or ‘Save Current Project’ menu item. Selecting the ‘Save Current Project As’ menu item will open a standard Windows file save dialog box. The current project is saved to the directory specified by the user by typing a name in the File Name field and clicking the Save Button. Clicking the Cancel button on the save dialog will take the user back to the NAS Main Menu screen without saving changes. Selecting the ‘Save Current Project’ menu item will save the project to the current specified *.nas file. If filename has not yet been specified, the ‘Save Current Project As’ function will be implemented.

Add Existing Project

To add the contaminant and redox indicator profile data sets from an existing *.nas file to the currently loaded *.nas file, select the ‘Add Existing Project’ menu item. NAS will automatically parse the additional data sets into the current projects contaminant and redox data set lists.

Contaminant Database

For data management and reporting purposes, NAS provides a database of contaminant sources that may be managed by the user, and may be accessed by selecting the ‘Contaminant Database’ menu item shown in Figure 5.

Export To Excel

Selecting the ‘Export to Excel’ sub-item opens a Microsoft Excel file listing all contaminant sources that are currently stored by NAS. The format for this file is shown in Table 3 in Appendix B. The database file is saved as ‘NASContDB.xls’ in the NAS Program Files directory.

Import From Excel

Users familiar with the format may manually edit the database file (e.g. adding additional contaminants groups) and then import it back into NAS. The user is advised to first make a backup copy before editing the database file.

Reload Default Database

If users develop errors in their database, or simply wish to revert back to the original database supplied with the current version of NAS, the user may select the ‘Reload Default DB’ sub-item.

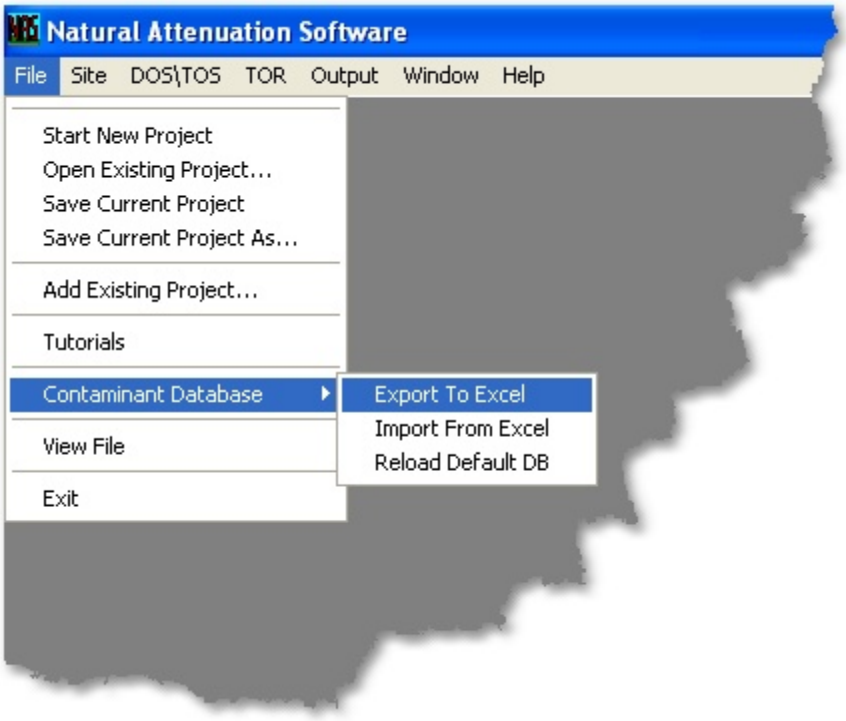


Figure 5. File – Contaminant Database Menu

Tutorials

NAS provides the user with example *.nas files in a 'Tutorials' directory in the NAS Project Files directory. To view a tutorial file, open NAS and select the 'Tutorials' menu item. A standard Windows file open dialog box will appear, in which you may select one of the example files in the 'Tutorial' directory. This action will take you to the 'General Tab' of the 'Site Data' Form. This form will be discussed in greater detail in a following section.

File View

NAS provides the user with a Microsoft Notepad-style file viewer shown in Figure 6. To view a text file, the user may select 'View File' menu item. A standard Windows file open dialog box will appear, in which you may select any text file (e.g. *.nas). You then have full Notepad functionality and may view, edit, change, and save the file.

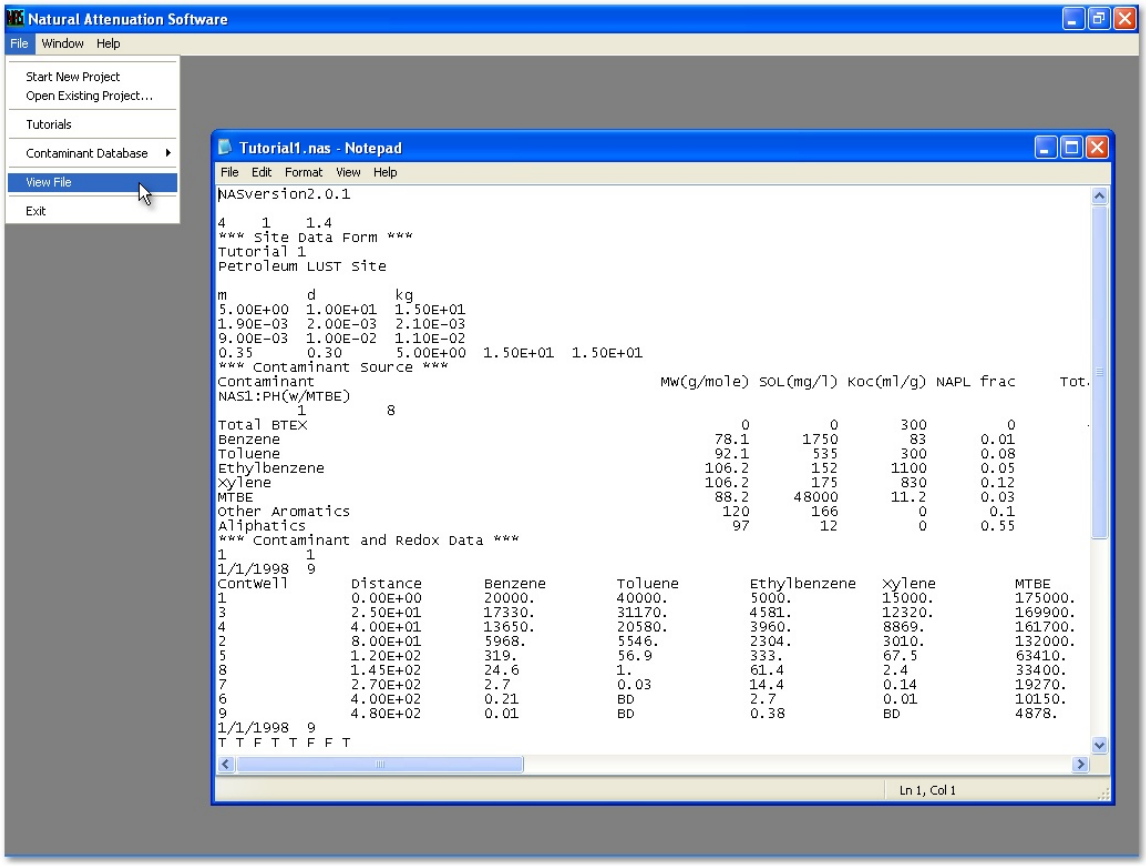


Figure 6. Notepad-Style File Viewer

Exit

Selecting the 'Exit' menu item will close NAS. If the user attempts to exit NAS without first saving the current project, NAS will prompt the user (via an informational message box) to make sure the user wishes to exit the project without saving changes.

Windows

The 'Windows' menu, shown in Figure 7, enables the user to arrange multiple forms within the main NAS Window. The lower part of the menu allows navigation to any NAS form open in the main Window.

Cascade

Select the 'Cascade' menu item to cascade all nonminimized forms.

Tile

Select the 'Tile' menu item to tile all nonminimized forms horizontally.

Arrange Icons

Select the 'Arrange Icons' menu item to arrange all minimized form icons.

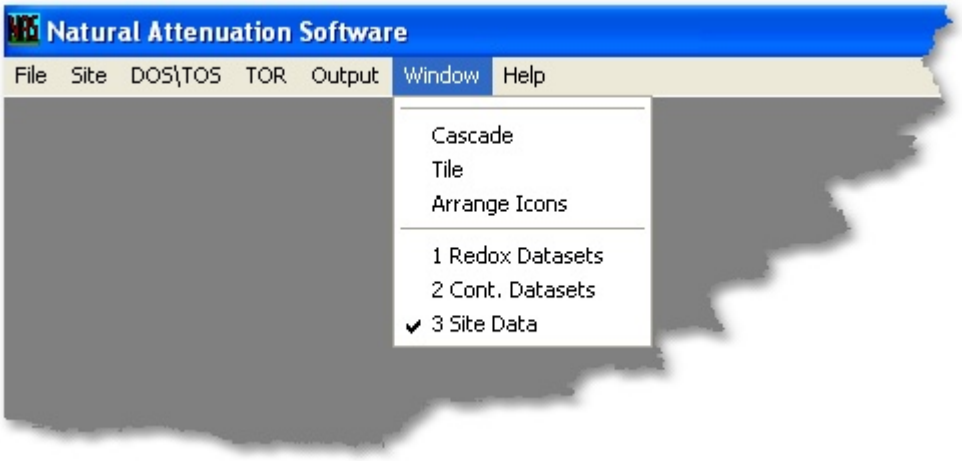


Figure 7. Window Menu

Help

NAS Help topics and useful information can be accessed through the 'Help' menu. See Figure 8 and Figure 9.

Documentation

The user may view the NAS User's Guide, and any other useful documentation that may become available, by selecting the 'Documentation' menu. See Figure 8.

NAS on the Web

The user may access the website developed to support NAS, by selecting the 'NAS on the Web' menu item. See Figure 8.

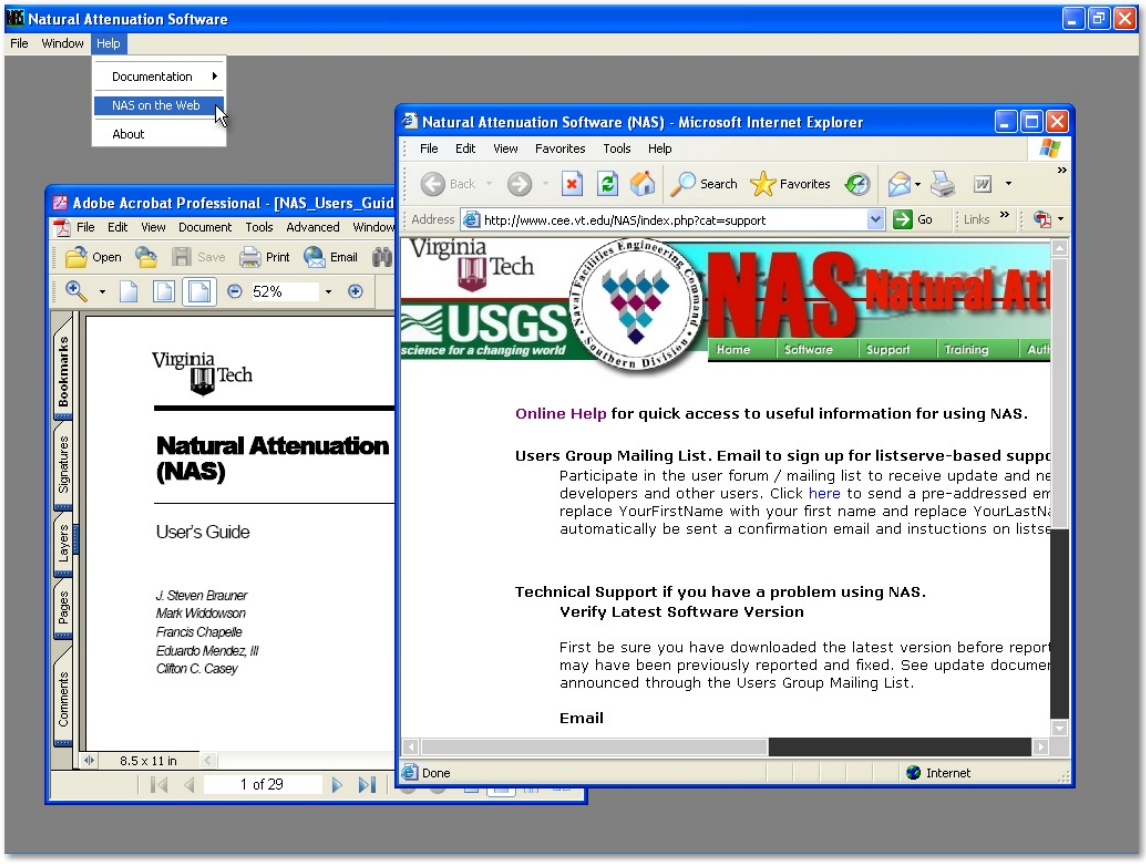


Figure 8. NAS Help

About

The 'About' menu item allows the user to review information about the authors, their contact information, and the current version of NAS. A 'System Information' button may also be clicked to provide system information that may be useful if it is ever necessary to contact NAS Technical Support. See Figure 9.

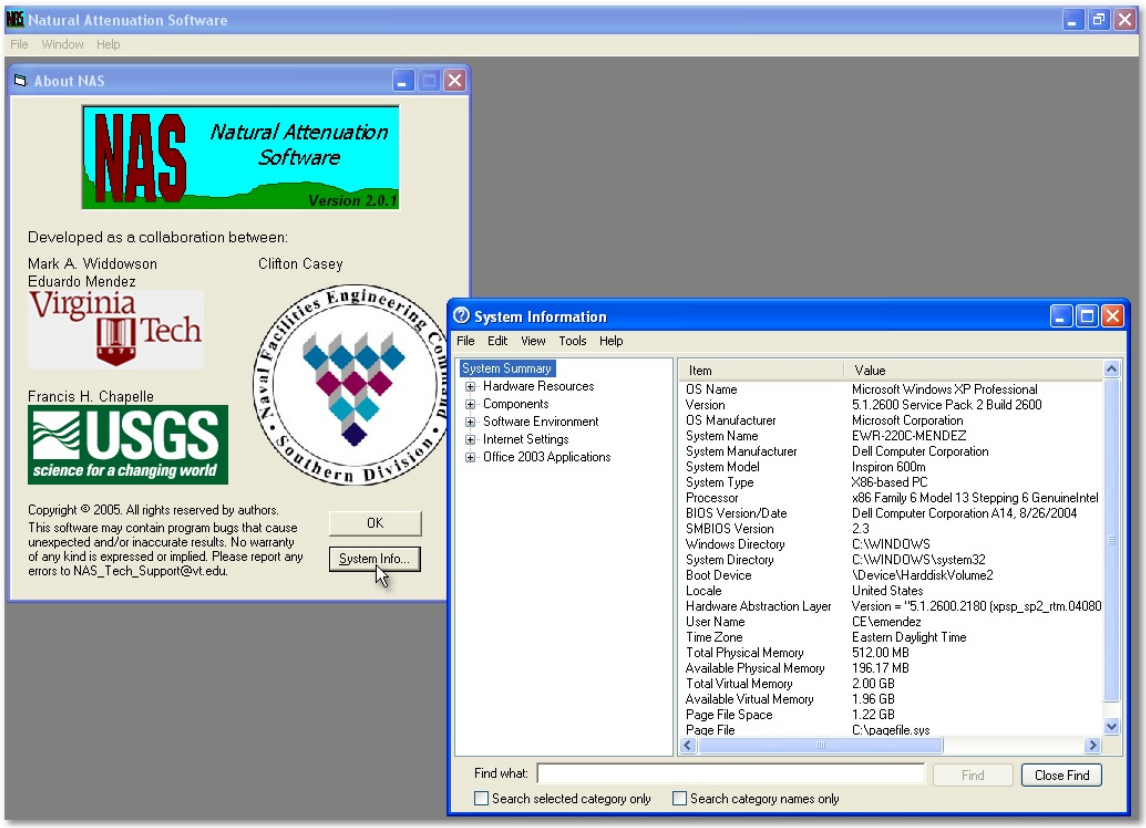


Figure 9. About NAS and System Information Screens

Site Data Assessment

Navigating the Site Data Window

Site data, including hydrogeologic parameters, contaminant source delineation and characterization, monitoring well locations, and concentrations of both contaminants and redox indicators, is entered using the Site Data form. The user is presented with a series of questions that are answered by the user via option buttons, check boxes, text boxes, or data entry. The user is required to enter all requested site data before performing any data analysis or source reduction/time of stabilization (DOS/TOS) or time of remediation (TOR) calculations (Note that the DOS/TOS and TOR program functions are disabled by NAS until all required site data has been entered.). Furthermore, the user is required to enter all requested data on a particular tab prior to NAS displaying the Next button that allows the user to proceed to the next tab. The user can always go back to change data that has been entered previously (by clicking on the appropriate tab to display the desired data entry field), but can not proceed to a new tab until all required information has been provided on the preceding tab.

To enter the site data entry window, start a new project or open an existing project, and then click on ‘Site’ menu on the NAS Main Menu screen. NAS automatically disables any tabs in which the user has not previously entered data.

Data Entry

General Data

The Site Data – General Tab prompts the user to (1) enter descriptive text for the identification of a particular site and (2) select units of measurement. See Figure 10.

Site Identification. Data entry for the descriptive text consists of a Facility Name, Site Name, and Additional Description for the new project. NAS does not require the user to enter information for any of these entries, as they are solely there for the benefit of the user in identifying a particular site or simulation.

Facility Name: User-specified text. Format: Character (up to 50 places). (Optional)

Site Name: User-specified text. Format: Character (up to 50 places). (Optional)

Additional Description: User-specified text. Format: Character (up to 50 places). (Optional)

Units Specification. NAS requires specification of units of measurement for length, mass, and time by choosing the appropriate option buttons. The selection of units of measurement will affect both the units displayed on screen for the various input and output variables used in NAS and any calculations based on empirical relationships that are unit-specific. The user should be careful to assure that values for all input variables are in the units specified by NAS. Failure to specify input values in the correct units may lead to erroneous calculations.

Length: User choice of meters or feet. Format: Option Button. (Required)

Mass: User choice of kilograms or pounds. Format: Option Button. (Required)

Time: User choice of days or years. Format: Option Button. (Required)

Concentration: NAS uses default units for concentration, as specified throughout the NAS interface.

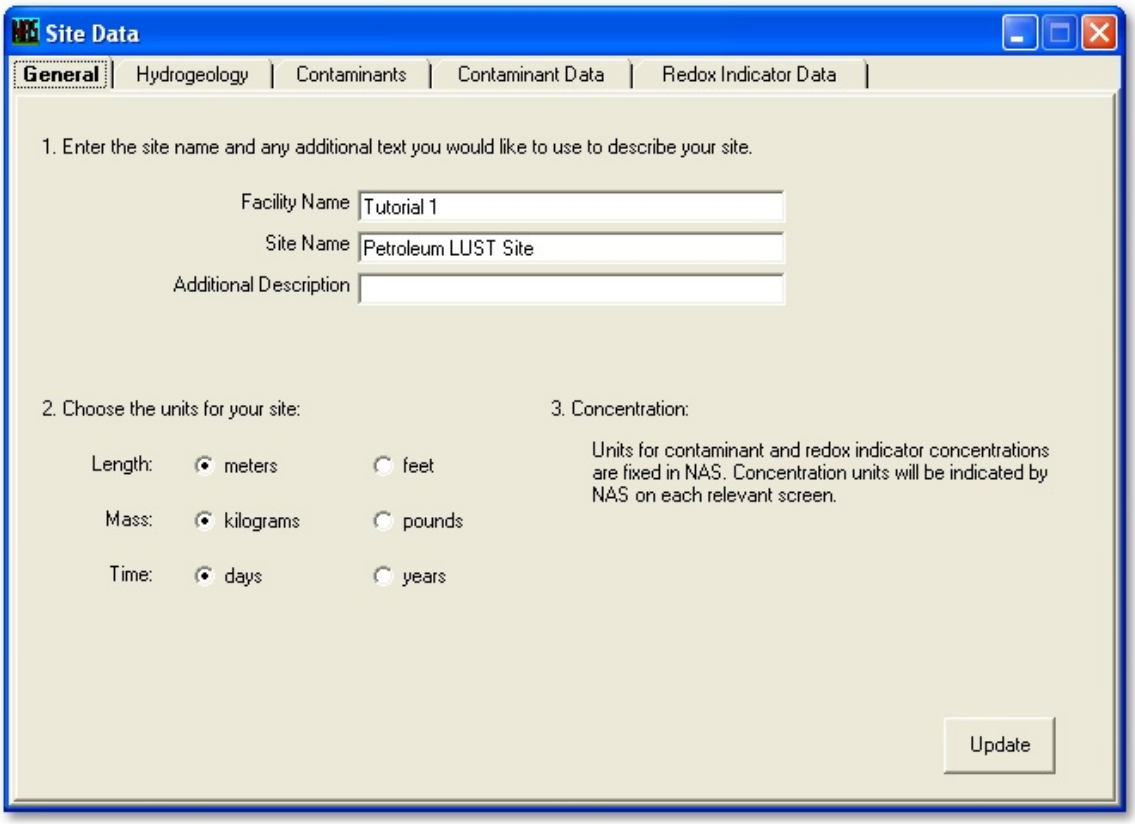


Figure 10. Site Data – General Tab

Hydrogeology

The Site Data – Hydrogeology Tab prompts the user to (1) enter values for hydrogeologic and aquifer properties and (2) delineate the contaminant source zone. See Figure 11.

NAS requires the user to enter the values for hydraulic conductivity, hydraulic gradient, weight percentage of organic carbon, porosity, and aquifer thickness. For the first three parameters, the user may enter a high, best, and low estimate. If a range of values is not available, enter the best estimate for all fields of each parameter. Note that NAS does not check the magnitude of these entries to insure that the user has entered these values in the correct order, so the user should take care to enter this data correctly. Hydraulic conductivity and hydraulic gradient values are used with the user specified porosity to calculate the high, best, and low estimate for groundwater velocity. These values are used to calculate high, average, and low first-order contaminant decay rates. The weight percent organic carbon values are used to calculate a range of distribution coefficients and retardation factors for each contaminant.

Hydraulic Conductivity: User entry of high, best, and low estimates. Format: Number greater than zero. (Required)

Hydraulic Gradient: User entry of high, best, and low estimates. Format: Number greater than zero. (Required)

Weight % Organic Carbon: User entry of high, best, and low estimates. Format: Number greater than zero. (Required)

Total Porosity: User enters best estimate. Format: Number greater than zero and less than one. (Required)

Effective Porosity: User enters best estimate. Format: Number greater than zero and less than one. (Required)

NAS requires the user to delineate the contaminant source zone by enter an estimate for the contaminant source length, width, and thickness. The width estimate is used in the 2-D analytical solutions for determining the concentration at a downgradient point based on a reduction in the source concentration, and the time of stabilization estimates. All three estimates are used in the 3-D numerical solution for time of remediation.

Source Length: User enters best estimate. Format: Number greater than zero. (Required)
Source Width: User enters best estimate. Format: Number greater than zero. (Required)
Contaminated Aquifer Thickness: User enters best estimate. Format: Number greater than zero. (Required)

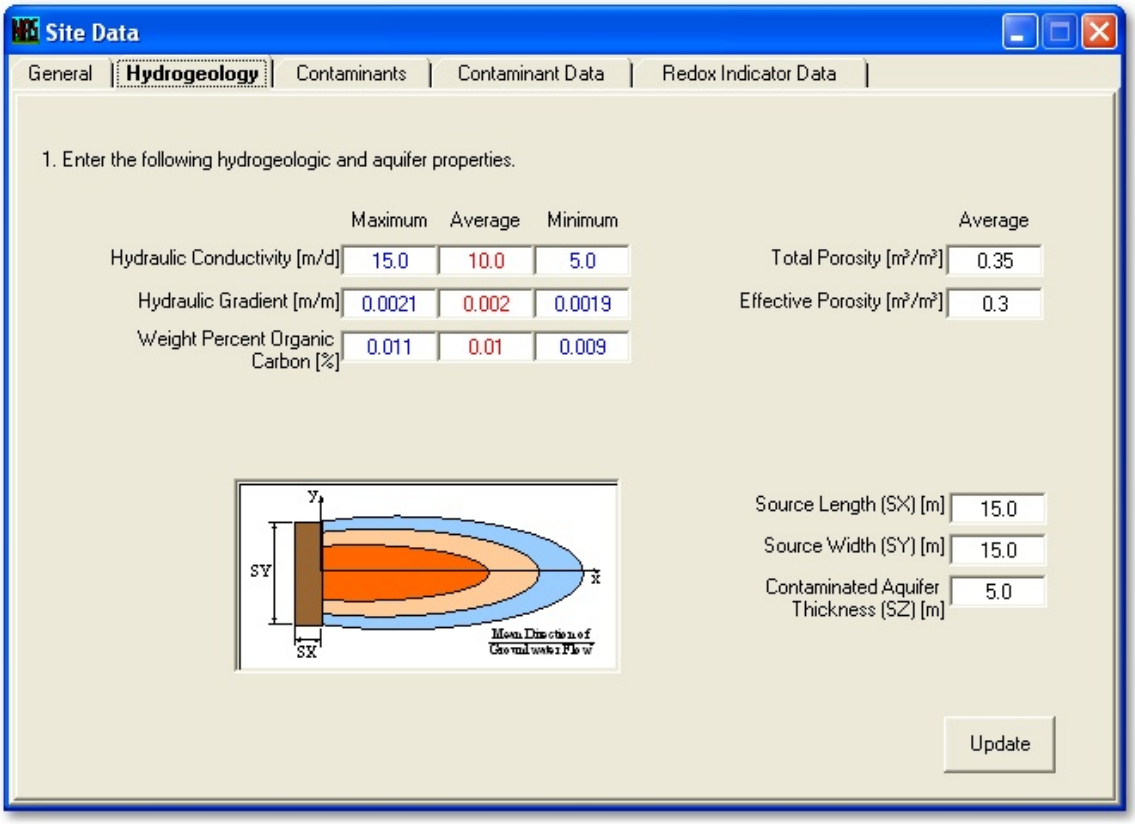


Figure 11. Site Data – Hydrogeology Tab

Source Contaminants

The Site Data – Contaminants Tab prompts the user to (1) specify the contaminant source constituents, and (2) specify values for contaminant properties required by NAS for the analytical and numerical solutions. See Figure 12.

The window on the left side of the form lists the contaminant groups available in the database. A following section of this document will describe how the user may manage the database, including editing existing groups as well as creating new user-defined groups. Groups prefixed by 'NAS1' are not editable and are required for NAS2 to properly read pre-NAS2 project files. The user may define the source by selecting groups from the window on the right, and/or by creating new ones. When the user is finished defining a new source, it may then be saved in the NAS database for use in future simulations.

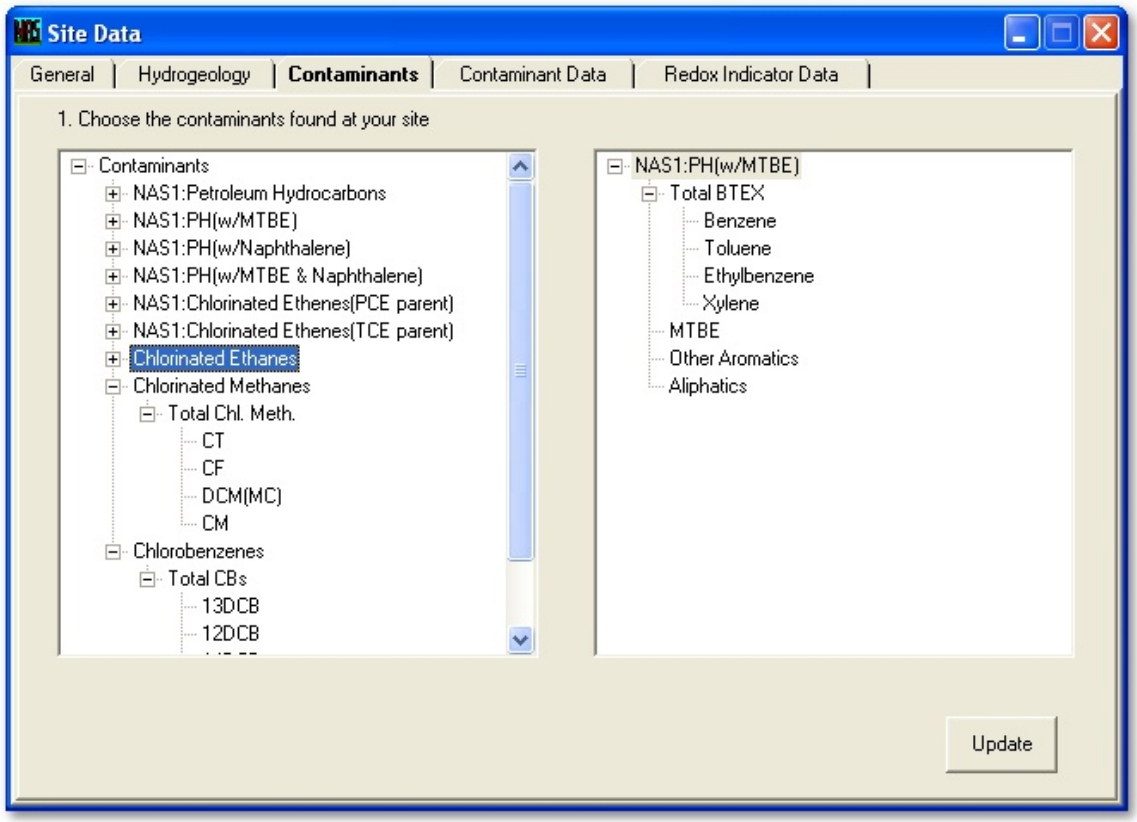


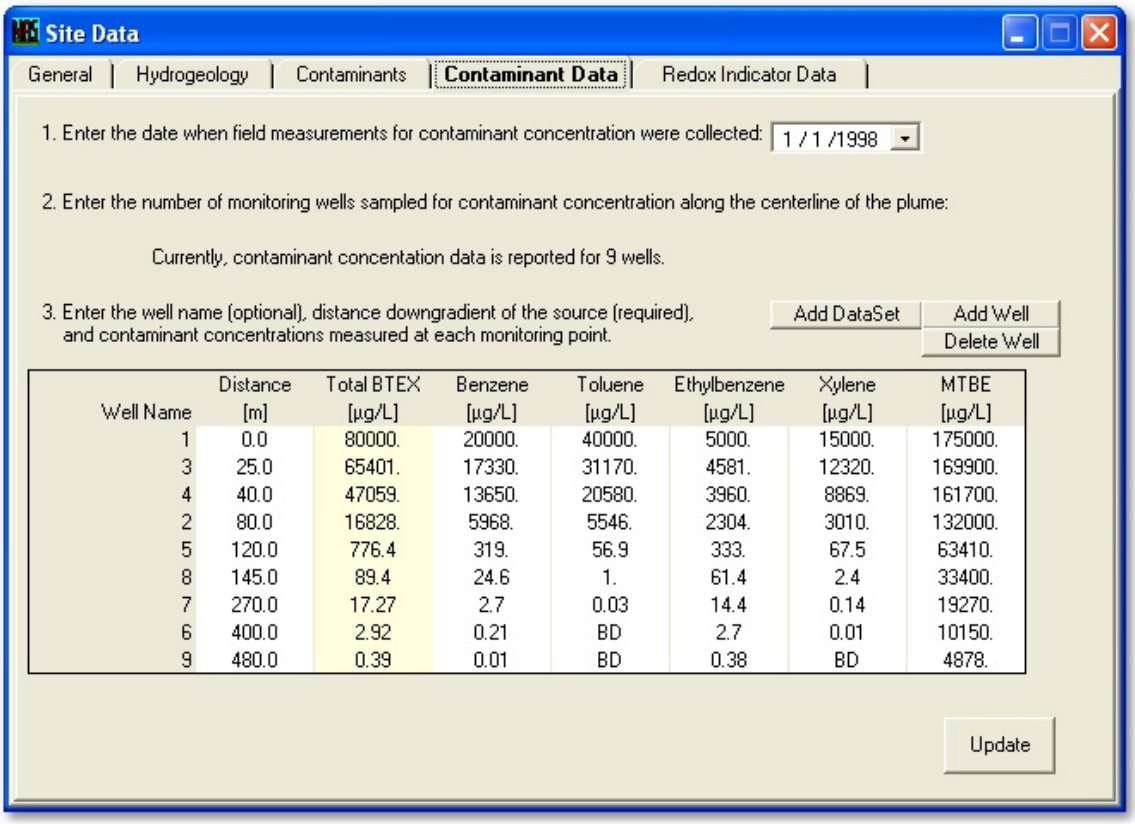
Figure 12. Site Data – Contaminants Tab

Contaminant Profile Data

The Site Data – Contaminant Data Tab prompts the user to (1) specify the date a contaminant profile data set was sampled, (2) specify the number of wells sampled for the data set, (3) specify the contaminant concentration profile, concentration versus distance from source, in tabular form, and (4) manage data sets by adding or deleting wells or data sets. See Figure 13.

NAS requires the user to enter the date the contaminant concentrations were sampled, the number of sample locations, the distance from the source to the contaminant well, and the contaminant concentration at each well. The date field, using a pop-up calendar, on the Contaminant Data tab is used to identify the data for convenience. The number of contaminant wells field is used to create the contaminant concentration data chart. The user is required to enter a number in this field when creating a new data site. The contaminant concentration data chart is then created using the Create Chart button. Note that the number of contaminant wells field disappears after the user clicks the Create Data button. It the user wishes to add or delete contaminant wells after creating the data chart, click the Add/Delete Wells button. The user may also add or delete a data set by clicking the Add/Delete DataSet button.

The contaminant data chart requires a distance from the source to the contaminant well and a contaminant concentration for each well. The distance from the source to the contaminant well should be measured from the front edge of the contaminant source and along the plume centerline. If data is unavailable for a particular contaminant at one or more wells, enter “NS” into the data chart (NS = Not Sampled). The NAS regression algorithm used to calculate Natural Attenuation Capacity (NAC) estimates for each contaminant will ‘skip’ NS entries. If a measurement is below detection, the user should enter “BD” into the data chart (BD = Below Detection). The NAS regression algorithm used to calculate NAC estimates for each contaminant will ‘skip’ BD entries if they are closer to the source than the maximum contaminant concentration, but will treat a BD entry downgradient of the maximum contaminant concentration as the furthest extent of the contaminant plume (independent of whether any above detection concentrations are entered downgradient of the BD entry). NAS does not require the user to enter a name for each contaminant well, but will store user names up to 15 places long.



Well Name	Distance [m]	Total BTEX [µg/L]	Benzene [µg/L]	Toluene [µg/L]	Ethylbenzene [µg/L]	Xylene [µg/L]	MTBE [µg/L]
1	0.0	80000.	20000.	40000.	5000.	15000.	175000.
3	25.0	65401.	17330.	31170.	4581.	12320.	169900.
4	40.0	47059.	13650.	20580.	3960.	8869.	161700.
2	80.0	16828.	5968.	5546.	2304.	3010.	132000.
5	120.0	776.4	319.	56.9	333.	67.5	63410.
8	145.0	89.4	24.6	1.	61.4	2.4	33400.
7	270.0	17.27	2.7	0.03	14.4	0.14	19270.
6	400.0	2.92	0.21	BD	2.7	0.01	10150.
9	480.0	0.39	0.01	BD	0.38	BD	4878.

Figure 13. Site Data - Contaminant Data Tab

Redox Indicator Data

The Site Data – Redox Indicator Data Tab prompts the user to (1) specify the date a redox indicator profile data set was sampled, (2) specify which redox indicators were sampled for in the data set, (3) specify the number of wells sampled for the data set, (4) specify the redox indicator concentration profile, concentration versus distance from source, in tabular form, and (5) manage data sets by adding or deleting wells or data sets. See Figure 14.

As with the Contaminant Data tab, the user is required to enter a date that the redox indicator concentrations were sampled. The user is required to enter oxygen, iron(II), and sulfate concentrations for each redox monitoring point, and may choose to enter data for nitrate, manganese(II), hydrogen sulfide, methane, or hydrogen by clicking the appropriate box on the Redox Indicator Data tab. The user must also specify the number of redox indicator monitoring points. The redox indicator monitoring points are initially specified as being the same well set as the contaminant wells. The user may, thereafter, add or delete wells by clicking the Add/Delete Wells button, and/or manually editing well names and distances. The user may also add or delete a data set by clicking the Add/Delete DataSet button.

NAS uses the user-specified redox profile with the Flowchart in Figure 38 in Appendix C, to delineate the redox zones at the site. If NAS is unable to identify a redox condition, at a particular well, that is in agreement with all provided redox indicator concentrations,

a ‘User Specification of Redox Condition’ dialog box will automatically appear and query the user for information. See Figure 15. For the case shown in the figure, the geochemical data indicates that aquifer condition at Well 4 is sulfate/carbon dioxide-reducing, whereas the hydrogen data suggests that the aquifer is ferrogenic. Since the geochemical data is not in agreement with the hydrogen data, NAS prompts the user to decide the redox condition. The user may also manually change any pre-determined redox condition by returning to the Redox Indicator Data tab and using the drop-down menu in the ‘Redox Condition’ column of the table to change the condition at the desired well.

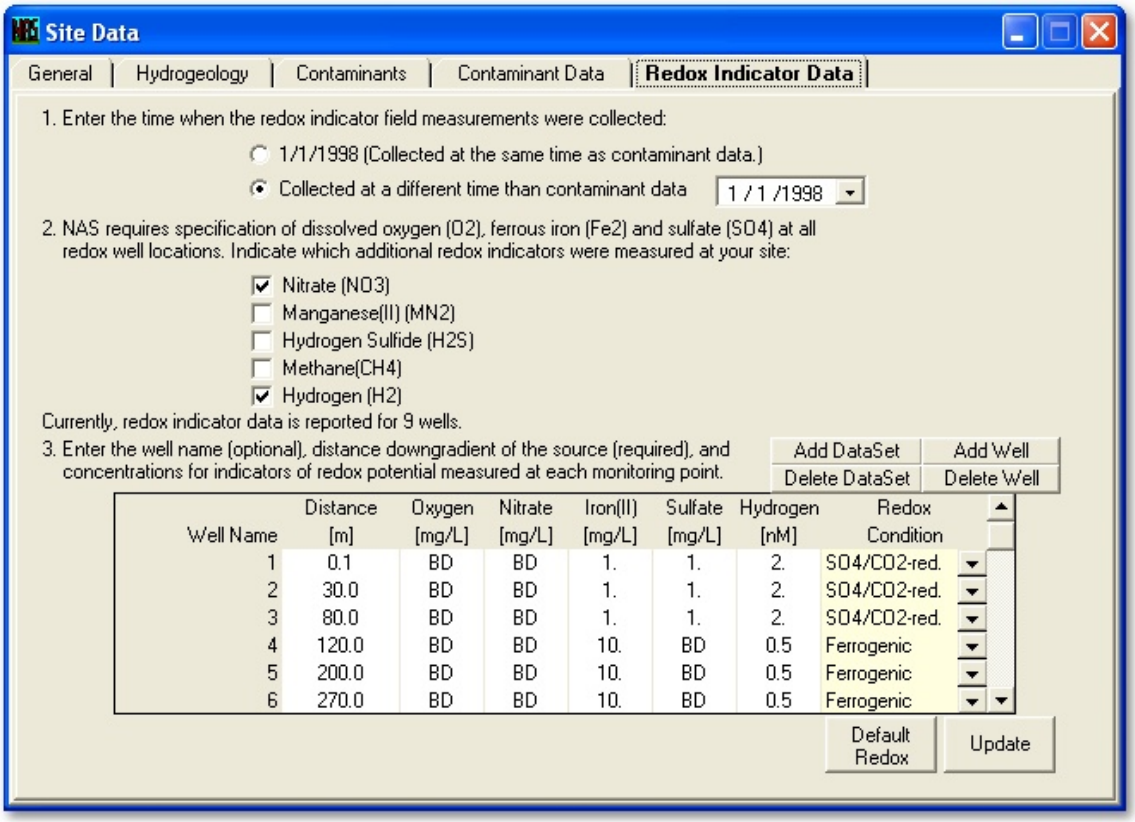


Figure 14. Site Data – Redox Indicator Data Tab

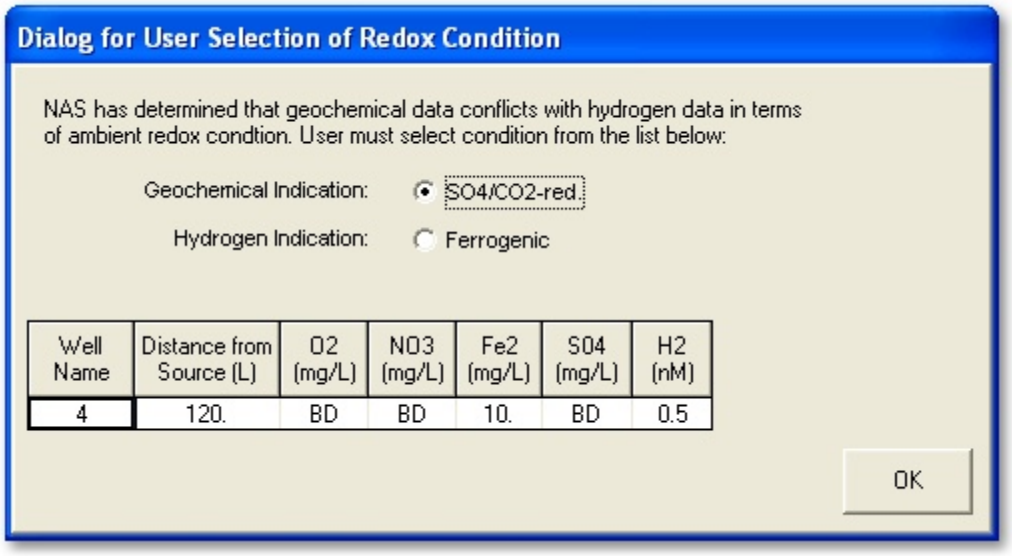


Figure 15. Dialog Box for User Selection of Redox Condition

Analyzing Output

Tabular Output of Site Data

Figure 16 contains an example of the tabular summary form that is created by NAS using the data entered in the Site Data form. NAS makes this form available if the user has progressed beyond the 'Site Data – General Tab'. The form may then be accessed through the 'Output -> Data and Results Tabular Summary' menu item. At the top of the form, a drop-down list is provided that quick-links to sections of the form. Sections include data input by the user and additional NAS-estimated values. Nas-estimated values for the table are based on the data sets currently selected in the Contaminant and Redox Dataset Lists. NAS-estimated values based on Site Data input are described as follows:

Groundwater contaminant velocity: Data from the Hydrogeology Tab is used to make high, best, and low estimates of groundwater contaminant velocity.

Sorption Data: Data from the Hydrogeology and Contaminants Tabs are used to estimate retardation factors for each contaminant.

Redox Zonation: Data from the Redox Indicator Data Tab is used to determine the redox zonation.

Natural Attenuation Capacity: Data from the Contaminant Data Tab is used to estimate Natural Attenuation Capacities (NACs) for each contaminant in each redox zone.

Dispersivity: Estimated NACs are used to determine the maximum plumelength. This maximum plumelength is then used, with a hardwired dispersivity ratio, to estimate longitudinal and transverse dispersivity values.

Decay Rate: Estimated NACs are used with estimated values for groundwater contaminant velocity and dispersivity to estimate decay rates for each contaminant in each redox zone.

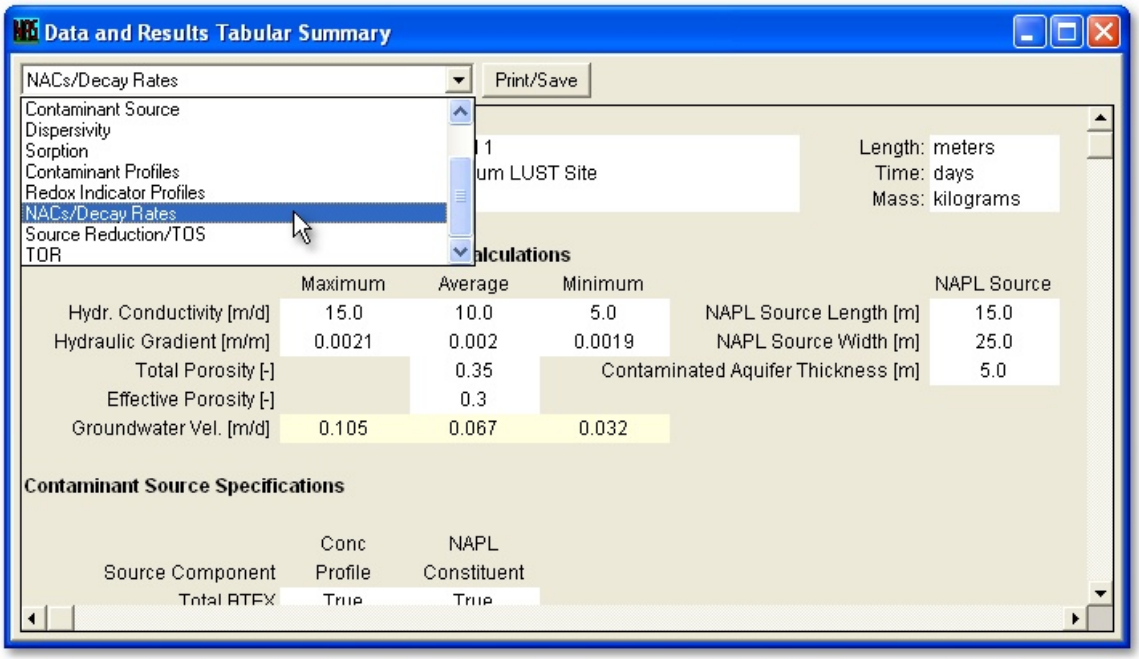


Figure 16. Tabular Output

Graphical Output of Site Data

Figure 17 contains an example of the graphical summary form that is created by NAS using the data entered in the Site Data form. NAS makes this form available when all of the required Site Data information has been entered. The form may then be accessed through the 'Output -> Site Data Graphs' menu item.

The graph displays the redox condition (as a function of space) through background shading and the user-specified concentrations as dots. The user can choose which contaminant to display using the pull down menu on the left. The user also can choose whether to hide a trendline, display the best-fit trendline, or display the multi-zone model trendline using the pull down menu on the right of the Graphical Summary tab. The user may view a trendline based on the data sets currently selected in the Contaminant and Redox Dataset Lists, or view trendlines for all contaminant datasets, against the currently selected redox dataset.

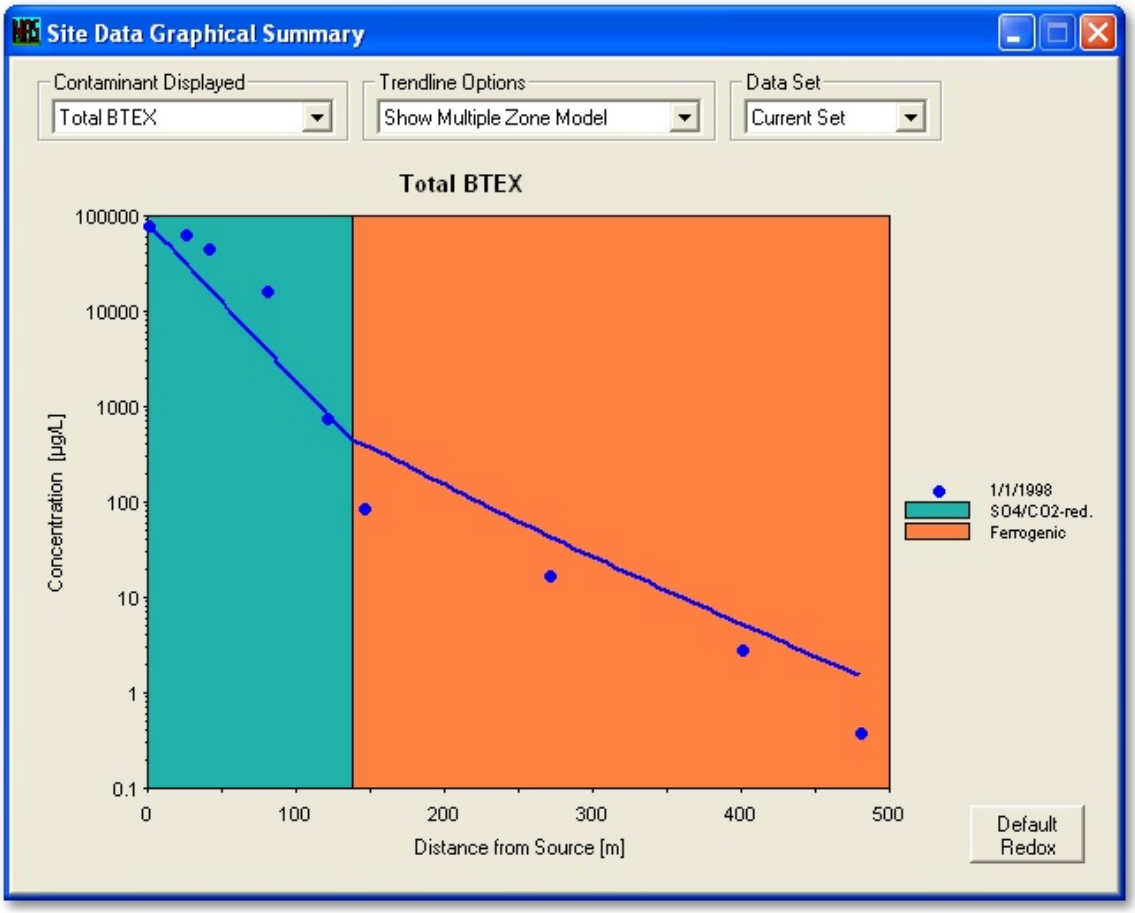


Figure 17. Graphical Output – NAC/Redox Zonation

Source Reduction and Time of Stabilization (DOS/TOS)

Navigating the TOS Window

NAS enables the user to estimate the reduction in the source concentration and time of stabilization (TOS) to reach a user-specified compliance concentration at a point downgradient of the source by clicking the Source Reduction / Time of Stabilization (DOS/TOS) menu on the NAS Main Menu. The Source Reduction and Time of Stabilization form, Figure 18, is a single window that does not require navigation, except to view the graphical solutions to a given problem.

Data Entry

Point of Compliance: The Point of Compliance (POC) is defined as the closest downgradient point of contact between a receptor and the contaminant of concern (e.g. property line, river, drinking water well).

POC at Well: A drop-down box is provided for the user to select an existing concentration well to represent the Point of Compliance.

Regulatory Compliance Concentration: The Regulatory Compliance Concentrations (RCC) is defined as the concentration of each contaminant at the POC that is acceptable for your site.

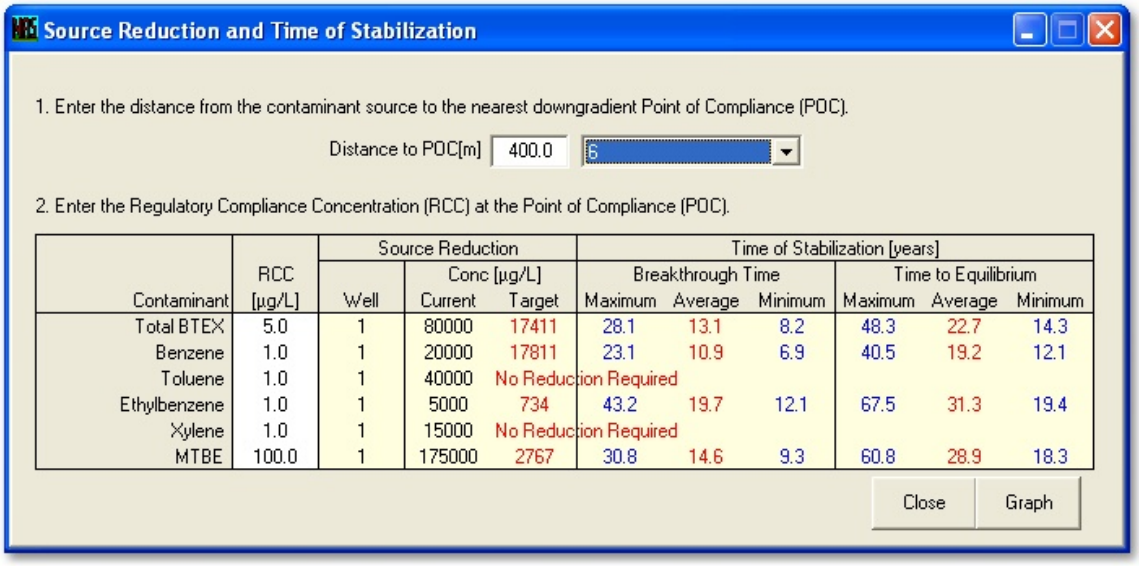
Analyzing Output

Tabular Output

Target Source Concentration: If NAS calculates that the RCC is exceeded at the POC, NAS estimates the target source concentration required to produce the specified RCC after source removal and plume restabilization. If the RCC is not exceeded for a give location, NAS will display 'No Reduction Required' in the Target Source Concentration column and will not calculate TOS values, as no Source Reduction is required for this case.

Time of Stabilization: If a source reduction is required, NAS provides the user with a range of Time of Stabilization (TOS) estimates. TOS estimates are based on the groundwater contaminant velocities and decay rates previously estimated by NAS. These estimates give the user an idea of how long after a source reduction an effect would be seen on concentration reduction at the POC.

> **Breakthrough Time:** NAS defines breakthough time as the point at which 50% of the required concentration reduction at the POC has been reached. High, best, and low values for breakthrough time are estimated.
>
> **Time to Equilibrium:** NAS defines time to equilibrium as the point at which the concentration has been reduced to approximately the RCC at the POC. High, best, and low values for time to equilibrium are estimated.



Contaminant	RCC [µg/L]	Source Reduction Well	Conc [µg/L] Current	Conc [µg/L] Target	Time of Stabilization [years] Breakthrough Time Maximum	Breakthrough Time Average	Breakthrough Time Minimum	Time to Equilibrium Maximum	Time to Equilibrium Average	Time to Equilibrium Minimum
Total BTEX	5.0	1	80000	17411	28.1	13.1	8.2	48.3	22.7	14.3
Benzene	1.0	1	20000	17811	23.1	10.9	6.9	40.5	19.2	12.1
Toluene	1.0	1	40000	No Reduction Required						
Ethylbenzene	1.0	1	5000	734	43.2	19.7	12.1	67.5	31.3	19.4
Xylene	1.0	1	15000	No Reduction Required						
MTBE	100.0	1	175000	2767	30.8	14.6	9.3	60.8	28.9	18.3

Figure 18. TOS - Input/Tabular Output Screen

Graphical Output

NAS provides graphical representations to the source reduction/time of stabilization solutions. The steady-state solution graphs, concentration versus distance, are based on the multiple zone model, if the simulation has more than one redox zone. The transient solution graphs, concentration versus distance, are based on the single best-fit NAC values to the POC. NAS also provides a 'TOS Concentration vs. Time Graph' which is a concentration versus time to stabilization graph at the POC. The graphs may be accessed by clicking on the 'Graph' button located on the bottom-right of the 'Source Reduction and Time of Stabilization' form, or if the user has already entered the required TOS data, through the 'Output -> DOS/TOS Graphs' menu item in the NAS Main window.

Steady-state solution graph

NAS provides a graphical view of the reduction in source concentration solution. Figure 19 shows the 'Steady-State Solution' Tab of the 'TOS Graphical Output' Form. This tab shows the Steady State solution (both existing and final) for the contaminants which may be selected from the drop-down list. Check boxes allow the user to turn marker lines on or off for the POC and RCC values.

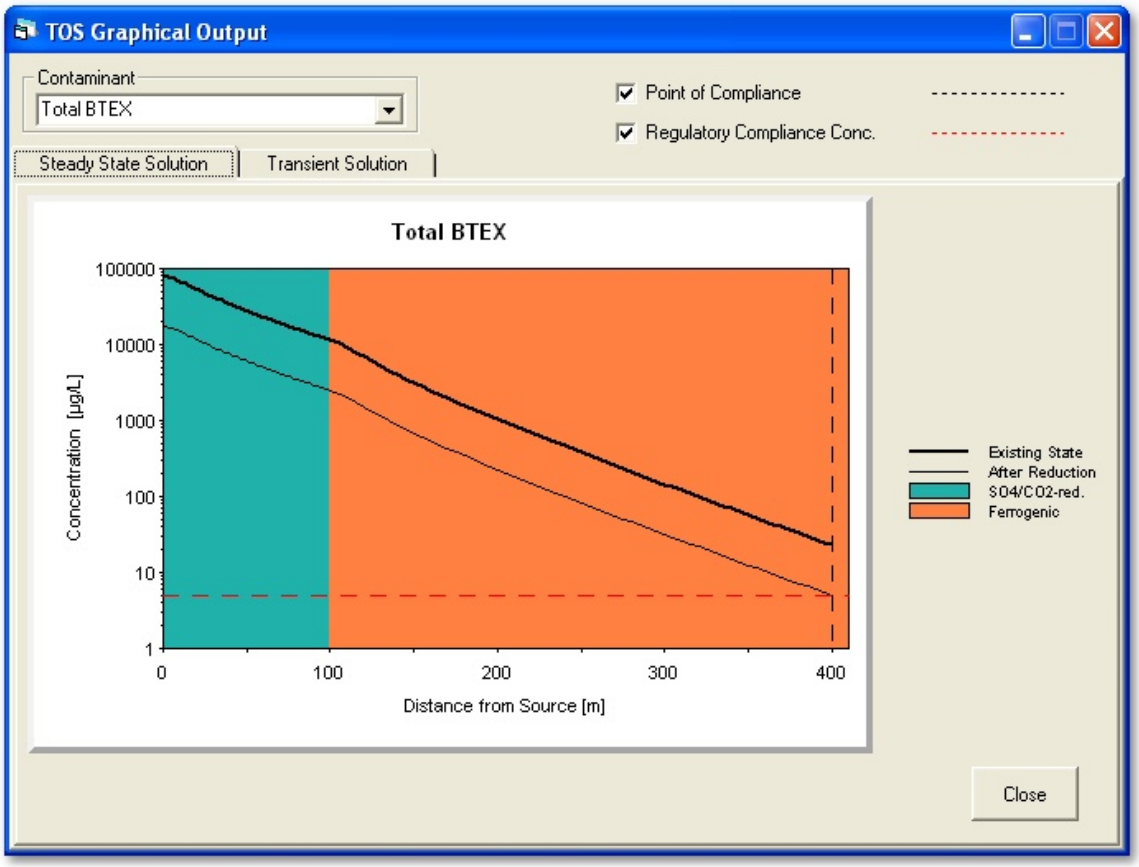


Figure 19. TOS – Graphical Output – Steady-State Solution

Transient solution graph

Figure 20 depicts the transient solutions to the same problem, which may be viewed by clicking on the 'Transient Solution' Tab of the 'TOS Graphical Output' Form. The solutions may be viewed for each contaminant selected from the drop-down list. Check boxes allow the user to turn marker lines on or off for the POC and RCC values. The >> and << buttons are used to move the transient solution timestep forward or backward one step in time, with the corresponding total period of time beyond source reduction being visible in the text box.

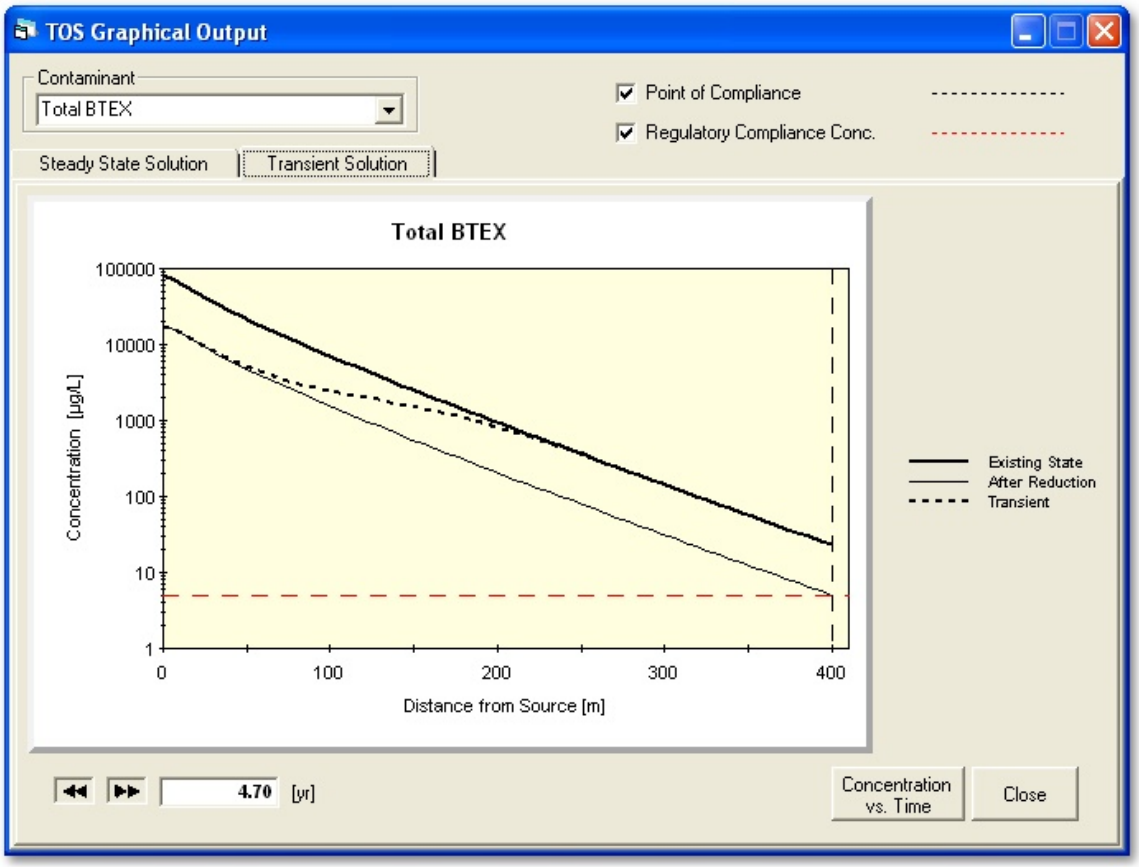


Figure 20. TOS – Graphical Output – Transient Solution

Concentration vs time graph

The 'TOS Concentration vs. Time Graph' shown in Figure 21 can be accessed by clicking the 'Concentration vs. Time' button on the 'Transient Solution' Tab of the 'TOS Graphical Output' Form. This graph is a concentration versus time to stabilization graph at the POC. A drop-down calendar is provided for the user to change the date of source reduction if different from the current concentration data set date. A checkbox enables users to toggle between viewing the low, best, and high TOS solutions based on the range in velocity. Another checkbox allows NAS-predicted versus monitored well points to be plotted; this is particularly useful if more than one contaminant dataset is included in the simulation.

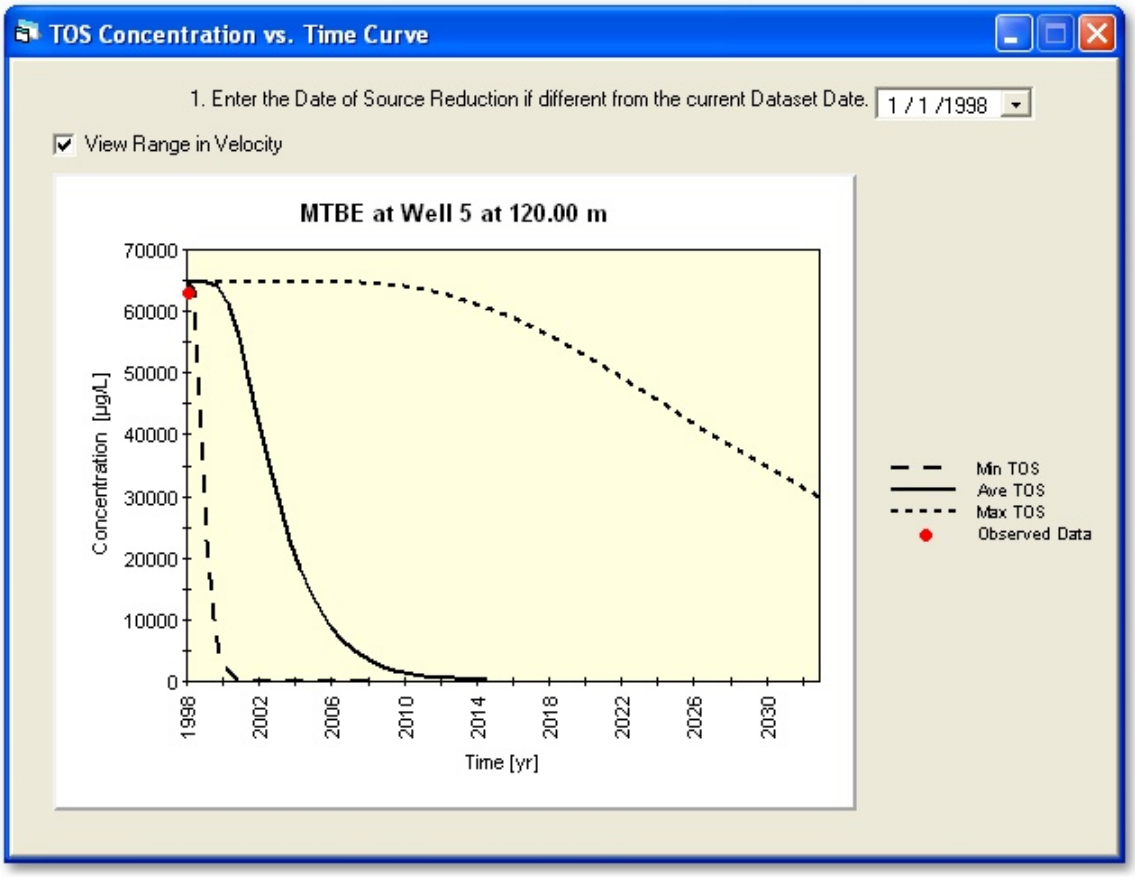


Figure 21. TOS – Graphical Output – Concentration vs. Time

Time of Remediation (TOR)

Navigating the TOR Window

Analysis for the Time of Remediation (TOR) requires the user to enter data and information needed to construct the input files for the SEAM3D numerical model. Note that time zero in the TOR analysis is the present or a future date at which NAPL source removal (partial or complete) has been implemented. The user enters NAPL properties, and an estimate (or estimates) for the NAPL mass through a series of tabs on the 'Time of Remediation' Form. The user is presented with a series of questions that are answered by check boxes, text boxes, or data entry. The user is required to enter all requested site data before performing TOR calculations. Furthermore, the user is required to enter all requested data on a particular tab prior to NAS displaying the Next button that allows the user to proceed to the next tab. The user can always go back to change data that has been entered previously (by clicking on the appropriate tab to display the desired data entry field), but can not proceed to a new tab until all required information has been provided on the preceding tab.

To enter the Time of Remediation form, click on the TOR menu item in the NAS Main window. NAS automatically takes the user to the tab that contains the last data entry.

Data Entry

NAPL properties

Figure 22 displays the NAPL Properties tab of the 'Time of Remediation' form. This tab includes contaminants from those specified by the user in the Contaminants tab of the Site Data form. The contaminants listed here are only those to which the user has assigned concentration profiles and/or specified to be in the NAPL source. The user may edit constituent properties (such as initial mass fraction) in this window, or the Site Data – Contaminants window, being sure to click the 'Update' button before saving or executing the simulation. Finally, NAS requires the user to specify the mass fraction of the NAPL for each compound. If one of the listed compounds is no longer found as a NAPL, enter zero for that compound. NAS requires the mass fraction of at least one constituent to be greater than zero. The sum of all NAPL mass fractions must be no greater than 1.0.

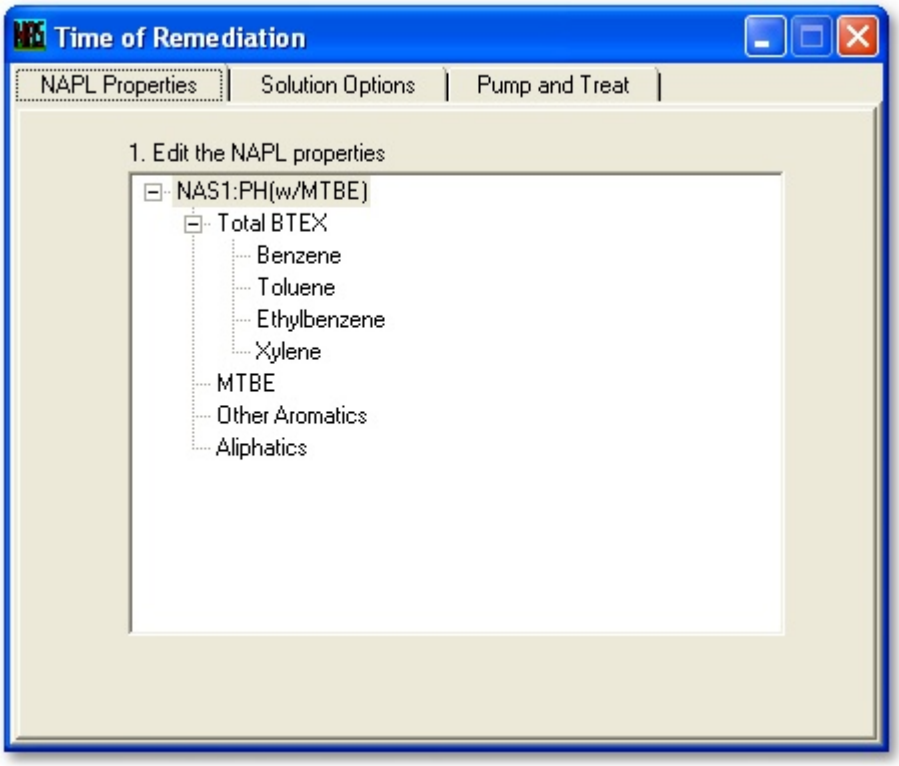


Figure 22. TOR – NAPL Properties Tab

NAPL Solution Options

Figure 23 displays the 'Solution Options Tab' of the 'Time of Remediation' form. This tab allows TOR estimates based on user-specified options for NAPL mass, source removal, range in velocity, and time of analysis.

NAPL mass options

NAS requires the user to specify at least one estimate for the NAPL mass and one remediation plan prior to performing the calculations necessary to estimate the TOR. The user may specify the current NAPL mass using one of the following options:

Best Estimate Only: The user is required to specify only one NAPL concentration.

Range of Values – Specify Minimum and Maximum: The user is required to specify three NAPL concentrations – a best estimate, a maximum, and a minimum

Range of Values – Use Percent of Best Estimate: The user is required to specify one NAPL concentration, and an estimate of how much variability is expected in this estimate.

Source removal options

The user may also specify up to three remediation plans, and is given the following options:

Estimate TOR if No NAPL Source is Removed: NAS will calculate the starting NAPL mass using the values specified in NAPL mass chart.

Estimate TOR for One NAPL Mass Removal Plan: NAS will calculate the starting NAPL mass by reducing the NAPL mass (or masses) in the NAPL mass chart by the percentage specified by the user. Note that entering zero for this plan is identical to the no source removal option above.

Estimate TOR for Two NAPL Mass Removal Plans: Same as the Estimate TOR for One NAPL Mass Removal Plan option, except the user may enter two NAPL removal percentages.

Estimate TOR for Three NAPL Mass Removal Plans: Same as the Estimate TOR for One NAPL Mass Removal Plan option, except the user may enter three NAPL removal percentages.

Velocity Range

A checkbox enables users to toggle between calculating TORs based on just the best estimate velocity, or to calculate with the range of TORs based on low, best, and high velocity estimates.

Simulation Time

The time of analysis is the simulation time the MODFLOW and SEAM3D numerical models are set to. The maximum time of analysis given to analyze the selected options is 100 years for each simulation. The simulation time for TOR analysis can be shortened by specifying a time of analysis that is less than the default (and maximum) value of 100 years. This option is exercised by changing the Time of Analysis field located at the

bottom of the Solution Options tab. It is advisable to do initial simulations with a lower analysis time, to prevent unnecessary runtimes.

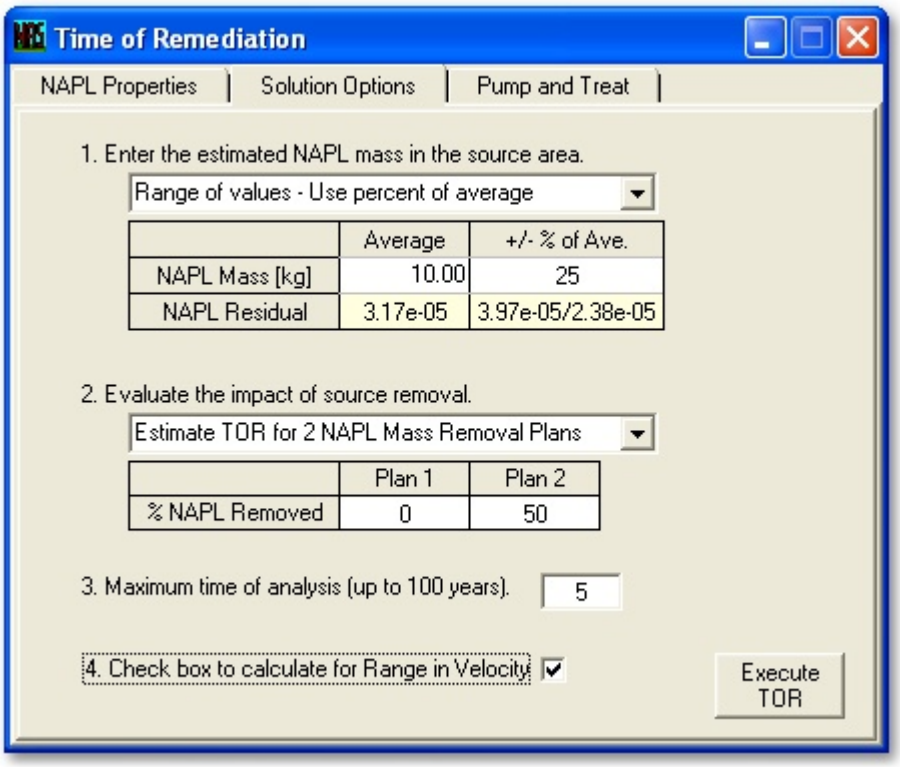


Figure 23. TOR – Solution Options Tab

Pump and Treat

Figure 24 displays the 'Pump and Treat' Tab of the 'Time of Remediation' form. This tab allows the user to estimate TORs associated with pump-and-treat technology for comparison with, or in conjunction with, MNA. NAS can model sites with an existing (or proposed) pumping well, or optimally design a pumping well field, with well location, pumping rate and duration, based on the previously specified site hydrogeology and source delineation data. If the 'Simulate Pump and Treat' checkbox is checked, NAS will simulate pump-and-treat for comparison with MNA. If pump-and-treat is simulated, required data includes:

Average Saturated thickness: A value for the average saturated aquifer thickness is required for the NAS estimate of pumping rate.

Pumping well distance: The distance from the source to the pumping well may either be specified by the user, or NAS will set it to the POC.

Pumping rate: The pumping well rate may either be specified by the user, or NAS will estimate it based on analytical solutions for hydraulic control and previously enter site data.

Pumping duration: The pumping duration may either be specified by NAS (in which case the pumping duration would be the total extent of the simulation time), or specified by the user (in which case it may be any value between zero to the total simulation time). If the pumping duration is less than the total simulation time, then the TOR simulation will consist of a pump-and-treat period followed by an MNA-polishing period for the remainder of the total simulation time.

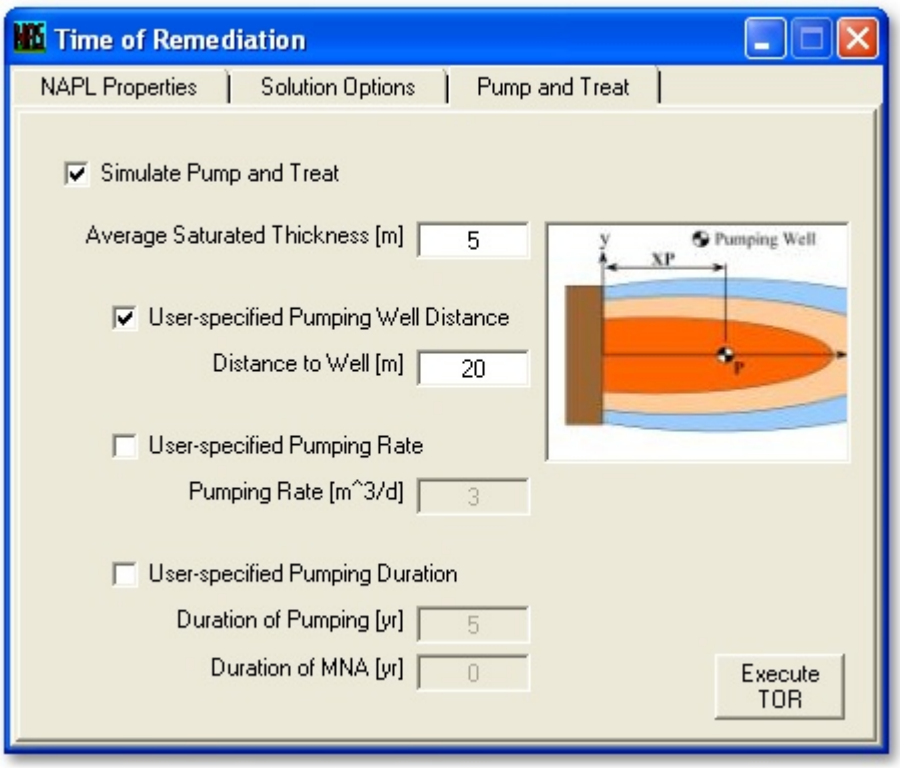


Figure 24. TOR – Pump and Treat Tab

Executing the TOR Simulation

When the user has completed specifying the solution options, the 'Execute TOR' button may be clicked on either the 'Solutions Options' or 'Pump and Treat' tab. This command initiates the MODFLOW and SEAM3D numerical solutions. The number of simulations that NAS will run is dependent on how the user specifies the NAPL mass, Remediation Plan, velocity range, and pump-and-treat options. The fastest TOR analysis, when SEAM3D is run only one time, is to specify a best estimate for the NAPL mass and only one remediation plan (either zero removal or a single percentage removal plan). The simulation time will reach a maximum when the user specifies a range of NAPL mass estimates, three remediation plans, velocity range, and pump-and-treat with MNA-polish period, which may require up to eighty-one separate SEAM3D simulations. Although this option will take more time, it gives the user more data to analyze for TOR estimates.

Figure 25 shows the 'Executing TOR' window that displays the progress of the TOR calculation. NOTE: If the calculation seems to have locked up due to an excessive amount of time, or you need to prematurely end the simulation, you may end the numerical model calculation buy closing its associated Microsoft-DOS window, that is minimized in the Windows Taskbar.

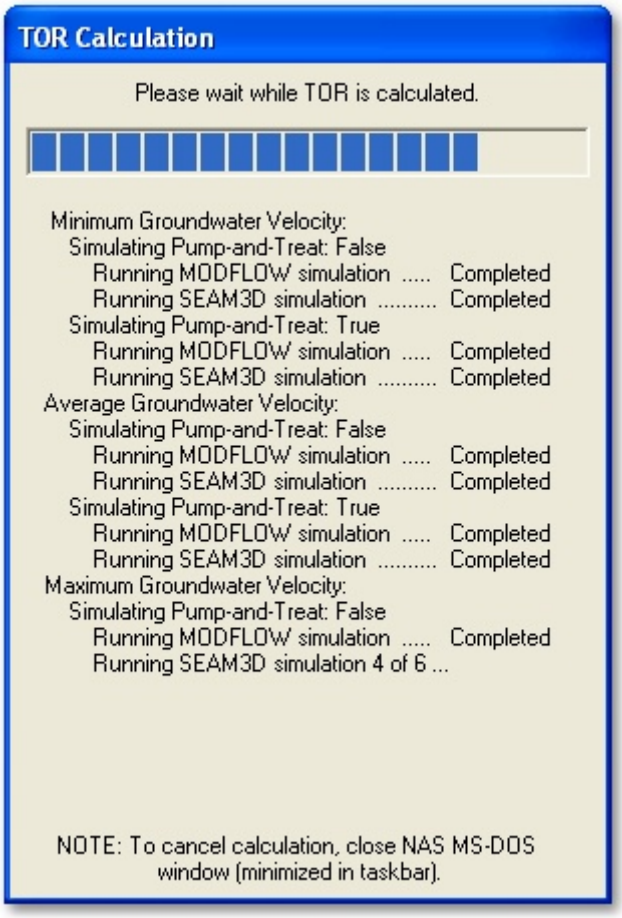


Figure 25. 'Execute TOR' Progress Dialog Box

Upon successful completion of the required simulations, a text file with the concentration versus time results is created with the same filename as the *.nas project file, and a file extension of *.obs. This file is created/saved in the same directory as the *.nas project file. These results then become available in the 'TOR Tabular and Graphical Output' Form which becomes visible after the simulation is complete.

Analyzing Output

The table and graph output for TOR will be automatically accessed immediately after a successful simulation run, or if the user has previously run a simulation, may be accessed through the 'Output -> TOR Table and Graph' menu item in the NAS Main window. This form provides drop-down boxes for the user to view results based on different contaminant, mass estimate, removal plan, velocity, and pump-and-treat options.

Time of Remediation Table

For NAS to calculate TOR, the user must specify the specified source compliance concentration (SCC) for each contaminant, on the 'TOR' Tab of the 'TOR Tabular and Graphical Output' Form. See Figure 26.

Source Compliance Concentration: The Source Compliance Concentrations (SCC) is defined as the concentration of each contaminant, at the source well (i.e. the first well), that is acceptable for your site.

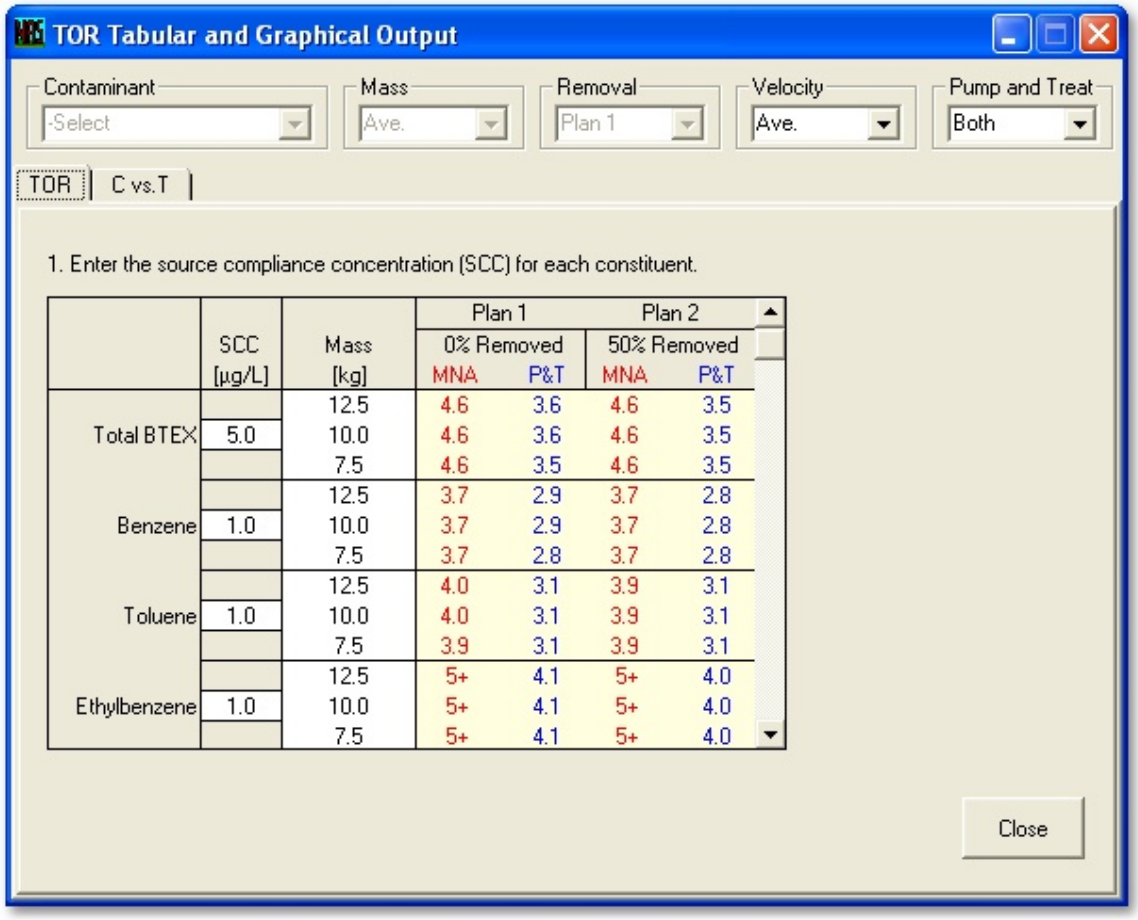


Figure 26. TOR – Tabular Output

Concentration vs time graph

NAS also offers a graphical representation of the TOR calculations based on the concentration versus time data contained in the associated *.obs file. The graph can be viewed on the 'C vs.T' Tab of the 'TOR Tabular and Graphical Output' Form. See Figure 27. A drop-down calendar is provided for the user to change the date of source reduction if different from the current concentration data set date. A checkbox allows NAS-predicted versus monitored well points to be plotted; this is particularly useful if more than one contaminant dataset is included in the simulation.

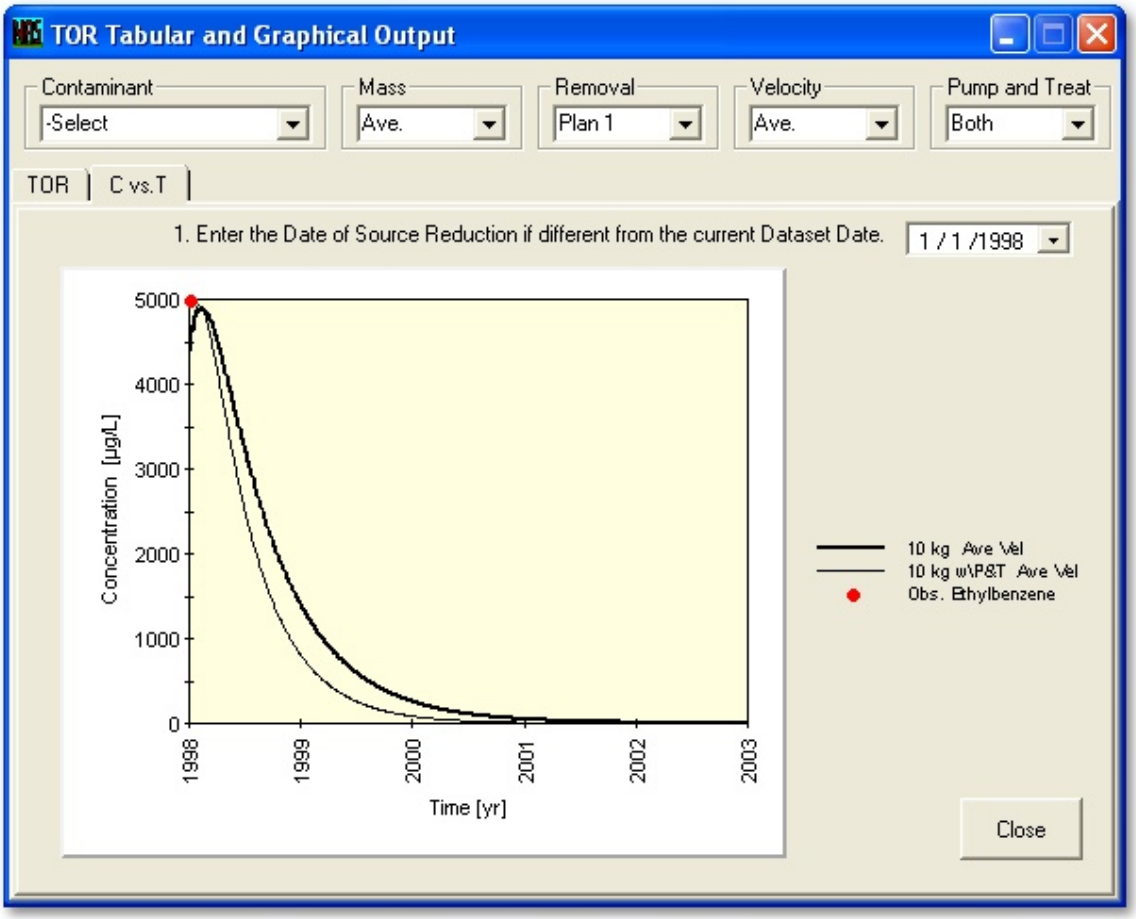


Figure 27. TOR – Graphical Output – Concentration vs. Time

Advanced Features

Adjusting Redox Zonation Graphically

In addition to being able to manually adjust the redox conditions in the 'Site Data – Redox Indicator Data' tab, NAS gives the user the ability to manually adjust the redox zonation from the 'Site Data Graphical Summary' form. The user can hover the mouse over redox zone boundaries, and when the mouse cursor changed to a double-header arrow, the user may click-and-drag the boundary in either direction. This may be useful when contaminant and/or redox indicator data is limited and slightly adjusting the boundary may better fit the observed data, and suggest where additional monitoring may be beneficial. As the user adjust boundaries, the impact on NACs can be immediately seen, and related estimates will be automatically updated in visible forms (except the TOR estimates which would require the numerical model to be executed again).

Managing Chronological Datasets

Contaminant and/or Redox Indicator data sets may be added to current projects either of two ways. One method was previously discussed in the NAS Main Menu section, by using the 'File -> Add Existing Project' menu item. This method is ideal if you already have NAS files made with the same monitoring profiles you wish to import, or if you

wish to import a NAS file that already has multiple datasets in it. Another method for deleting sets, or sequentially creating new ones, in a current project is with the 'Add/Delete DataSet' buttons in the 'Contaminant Data' and 'Redox Indicator Data' tabs in the 'Site Data' form. To delete a data set, highlight it in the corresponding 'Cont. Datasets' or 'Redox Datasets' list, and then click the corresponding 'Delete DataSet' button. To add a data set, select your existing data set that most resembles the data set you wish to add (i.e. the set with the date, number of wells, well names, and distances that most closely matches the set you are adding), and click the corresponding 'Add DataSet' button. You will then be prompted to select a date for the new set from the drop-down calendar. NAS will create a new concentration profile chart have the same number of wells, well names, and well distances of the data set you copied, and you will just be required to fill in the concentration values. Individual wells may still be added or deleted by the usual method if so desired.

Contaminant Database

Three types of items may be represented in the contaminant database: Contaminant Groups, Contaminant Totals, and Contaminants. The three items and how to edit existing ones or create new ones will be discussed in the following sections. NOTE: See Appendix A and Appendix B for additional information on required contaminant parameters and their definition and format.

Figure 28 shows the menu list that is accessed by opposite-clicking in the left window (Database window) of the 'Contaminants' tab of the 'Site Data' form. If clicked over an item (such as a contaminant group in this figure), the first menu item will add that item to the user-specified source zone window on the left. The next four menu items are available in both the Database window and the Source window, with the first three of these being self-explanatory. The fifth menu item 'Delete' will only be available when the use has clicked on an item, with the item name changing depending on which item the user may have clicked on. By clicking on the 'Update Contaminant Database' menu item, the user will revise the NAS internal contaminant database, with any changes being available to all future simulations of NAS.

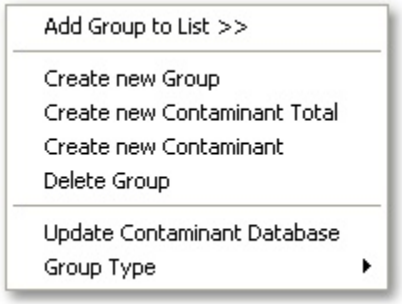


Figure 28. Database Window Menu Items

Figure 29 shows the menu list that is accessed by opposite-clicking in the right window (User-specified source window) of the 'Contaminants' tab of the 'Site Data' form. The only menu items singular to this window are the two with the left-facing arrows. Clicking on the 'Create New Group In Database' menu saves a copy of the user-defined

source group to the NAS database. Clicking on the 'Update Group In Database' menu revises a contaminant group in the database window with that of the same name in the source window.

Figure 29. Source Window Menu Items

To create a new contaminant source, one should first create a contaminant group, then add only contaminant totals or contaminants under it. To create a new contaminant total, one should only add individual contaminants under it. To create a co-mingled source, one should first create a contaminant group, classify it as 'Co-mingled', and then up to one of each of the other groups may be created/added within it.

Contaminant Group: The contaminant group item is a collection of contaminant totals and/or individual contaminants. Figure 30 is a view of the menu that becomes available when opposite-clicking on a contaminant group in the 'Contaminants' tab of the 'Site Data' form. The 'Group Type' submenu lists the types a group may be classified as. All contaminant totals and individual contaminants within a group will be classified as this type of contaminant. NOTE: If a group is classified as 'Co-mingled', it may then have, at the most, one of each other group (i.e. Non-reactives, Electron Donors, Electron Acceptors) in it.

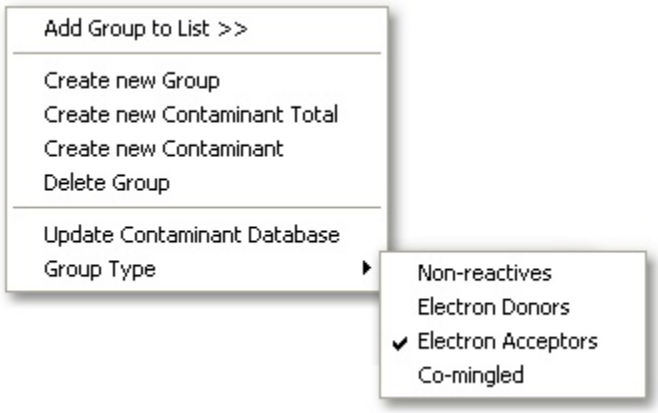


Figure 30. Contaminant Group Menu Items

Contaminant Total: The contaminant total item is a collection of individual contaminants. Contaminant totals will not be explicitly simulated in NAS, in that the user will not be required to enter concentration profile data for the item. NAS will sum the concentrations of the individual contaminants within the contaminant total, and use that value for calculations. Figure 31 is a view of the menu that becomes available when

opposite-clicking on a contaminant total in the 'Contaminants' tab of the 'Site Data' form. The 'Edit Properties' submenu produces the properties box as shown. The only required property for a contaminant total is:

Carbon Matter Partition Coefficient – Koc

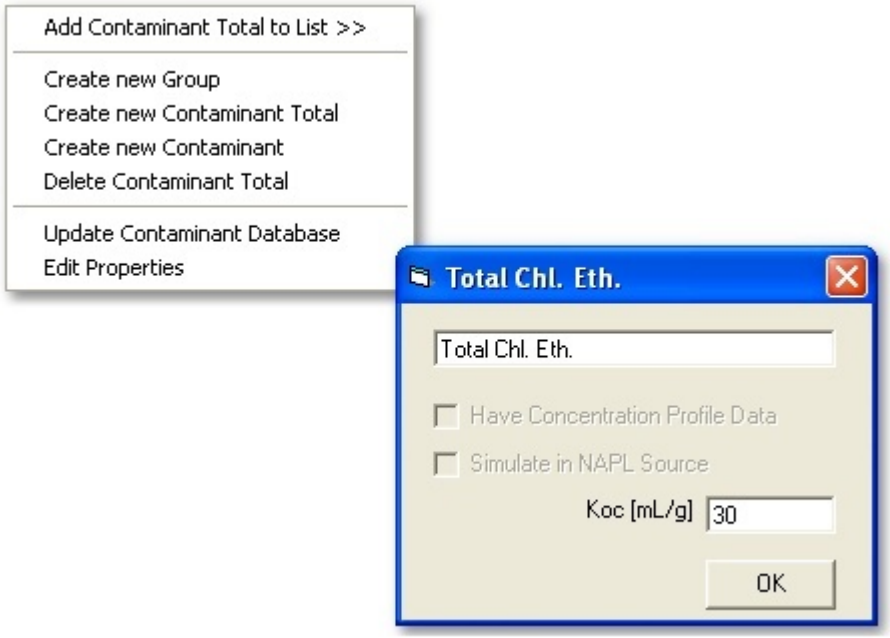


Figure 31. Contaminant Total Menu Items

Contaminant: The contaminant item is an individual contaminant. Figure 32 is a view of the menu that becomes available when opposite-clicking on a contaminant in the 'Contaminants' tab of the 'Site Data' form. The 'Edit Properties' submenu produces the properties box as shown. The user may use the checkboxes to specify if a concentration versus distance profile will be supplied, and if the contaminant will be simulated as a NAPL source constituent in the TOR simulation. The required properties for a contaminant are:

If 'Have Concentration Profile Data' or 'Simulate in NAPL Source' is true:

Carbon Matter Partition Coefficient – Koc

If 'Simulate in NAPL Source' is true:

Mass Fraction
Solubility
Molecular Weight

If 'Simulate in NAPL Source' is true, and 'Group Type' is 'Electron Acceptors':

Stoichiometric Factor
Alternate Pathway (see next section)

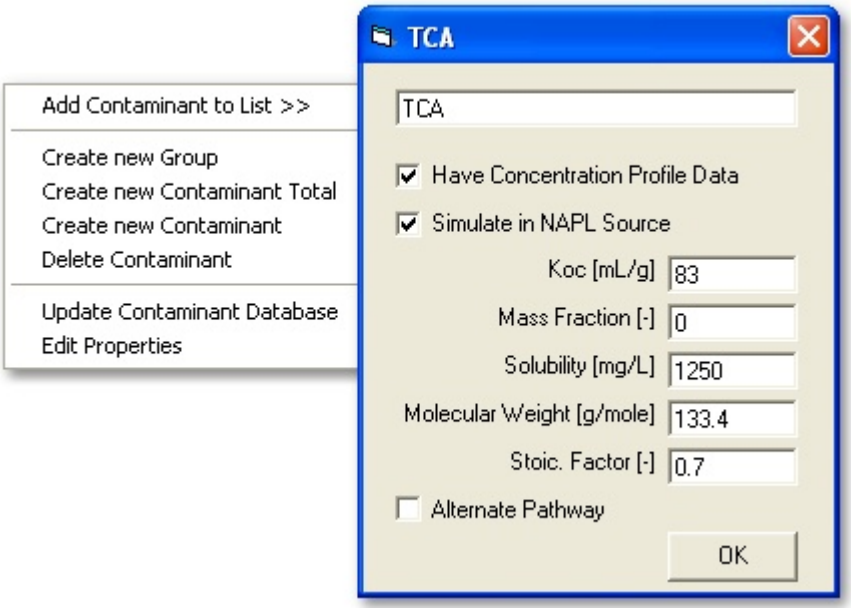


Figure 32. Contaminant Menu Items

Alternate Pathways:

If 'Simulate in NAPL Source' is true, and 'Group Type' is 'Electron Acceptors', then alternate reduction pathways may be specified. Figure 33 is a view of the additional data that is required when the user selects the 'Alternate Pathway'. These are:

Alternate Pathway Parent
Contaminant Percent from Parent

Figure 34 shown an example application of the alternate pathway function. The 'electron acceptors' contaminant group must be specified using a linear sequential pathway, such as that represented by Reductive Dechlorination in the figure. In this pathway, the parent may only go to one daughter product, with each daughter being the next parent in sequence. The alternate pathway function allows the user to specify additional child pathways from a parent, such as the abiotic degradation pathways shown in the figure.

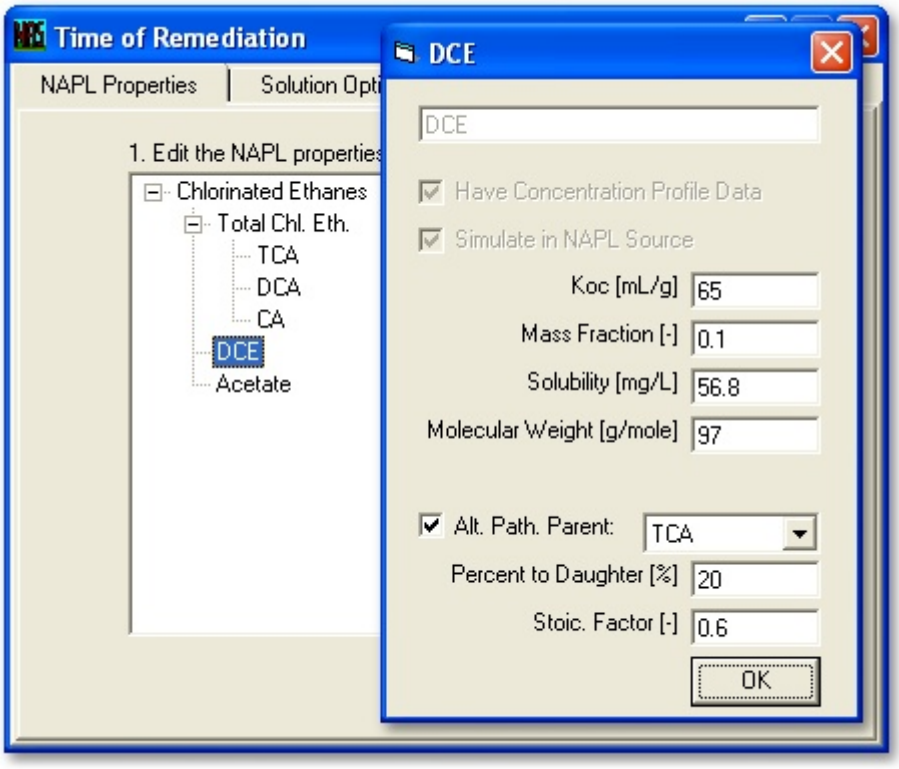


Figure 33. Specifying an alternate reduction pathway

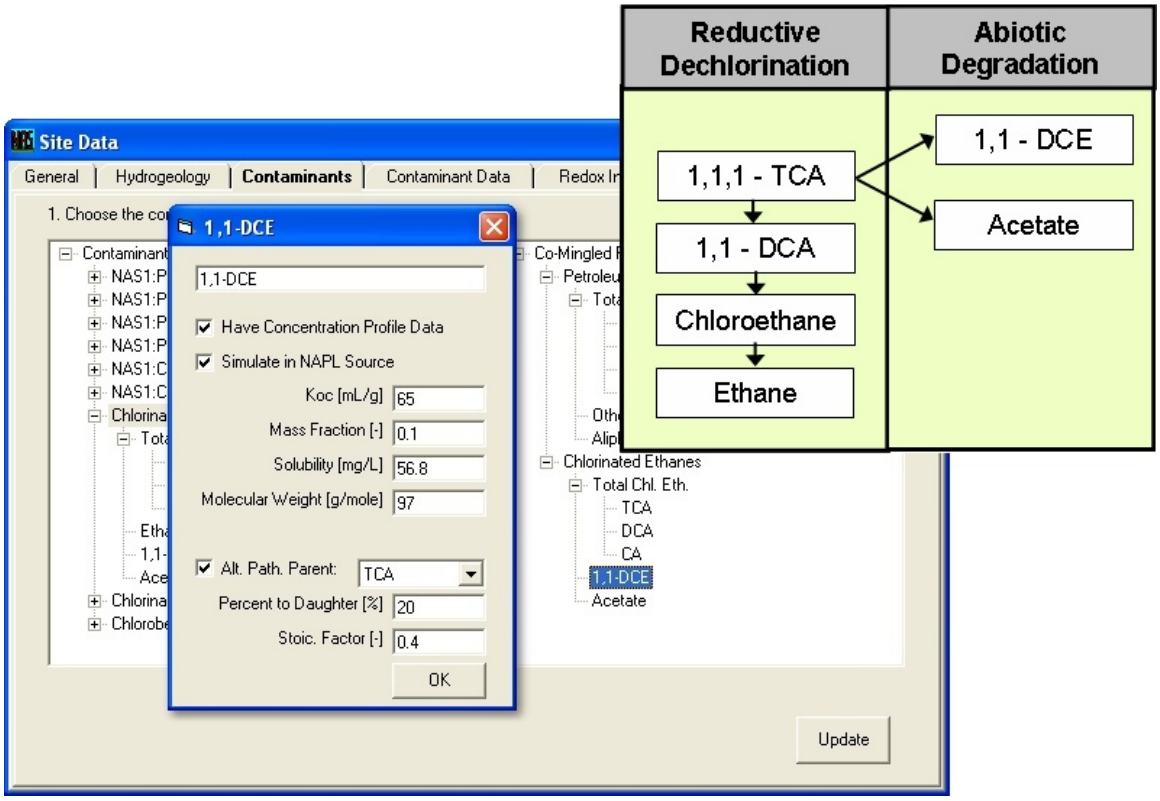


Figure 34. Example of Alternate Pathway Application

Reporting Features

Report Generation

Clicking on the 'Print/Save' Button on the 'Data and Result Tabular Summary' Form converts the form into a Print Preview report capable of being formatted, saved, and printed. See Figure 35. From the Print Preview, the following options are offered:

Navigation: The user can navigate through the data summary using either the Next/Previous navigation buttons, the Page Down/Page Up keyboard commands, or the scroll bar located to the left of the print preview.

Save: Clicking the Save button produces a standard windows save as dialog box enabling the user to save the Report in Excel file format.

Print: Clicking the Print button takes the user to a standard windows print dialog that allows the user to select the print range, select between various print options, and enter the print setup dialog. Once the user has selected the desired print range and options, the user may then choose to Print the selection.

Setup: Clicking the Setup button allows the user to simultaneously modify the print preview and options for the document sent to the printer. Among the options offered are margin widths, page orientation, custom headers/footers, and the on-screen zoom scale.

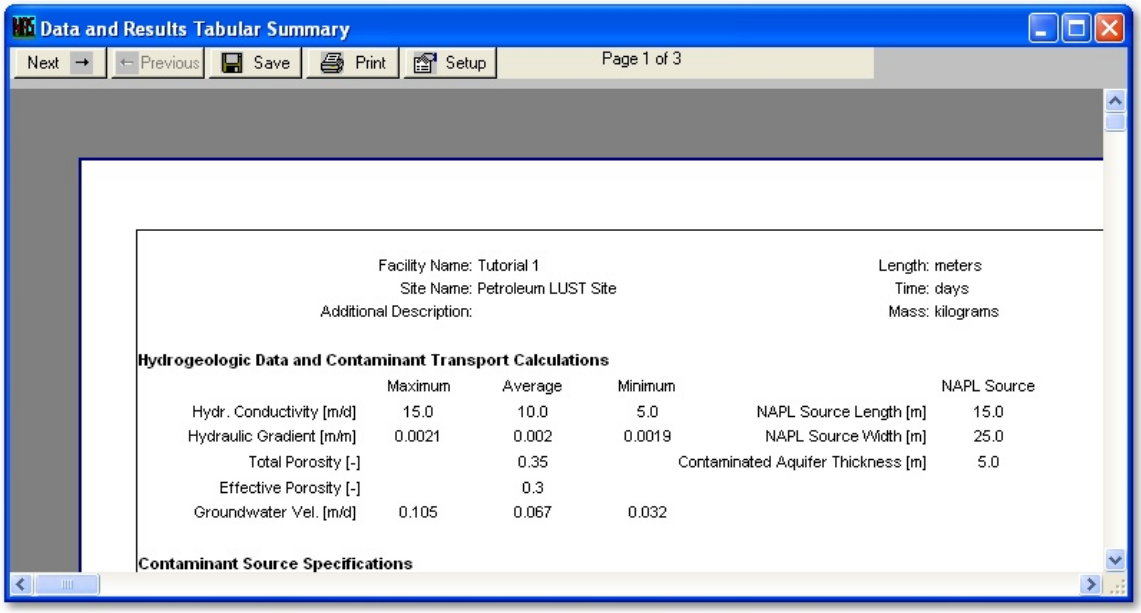


Figure 35. Report Generator provided for Main Tabular Output

Clipboard copy Tables

All tables in NAS have the capability of full Clipboard copy, for the purpose of pasting in reports. Select input tables in NAS also support pasting into them from the Clipboard (e.g

copying and pasting large blocks of data from an excel file into the Contaminant Data profile table).

Edit Graph Properties

All graphs in NAS, when opposite-clicked on, provide an editable properties dialog box. The user is given complete control to manage all visual aspects of the graph for reporting purposes. An associated help file can be accessed by clicking on the 'Help' button on the bottom right of the properties box. See Figure 36.

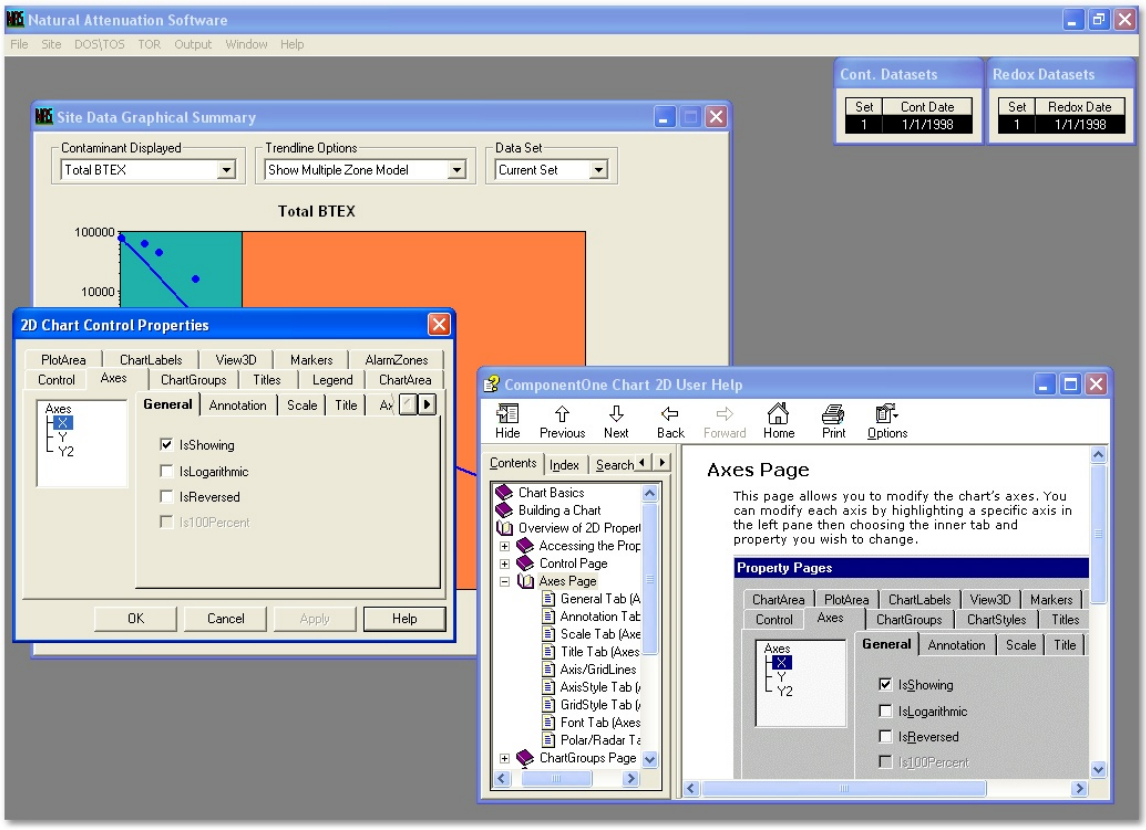


Figure 36. Graph Properties Dialog Box and Associated Help Screen

Save/Print Graphics

All graphs in NAS, when double-clicked on, provide a drop-down menu giving print and save options. Graphics can be printed in three different formats. Graphics can also be saved to either the Clipboard or a file in three different formats each. The 'Set Report Format' may be used to make the graphic more friendly for low-color or black-and-white reporting. See Figure 37.

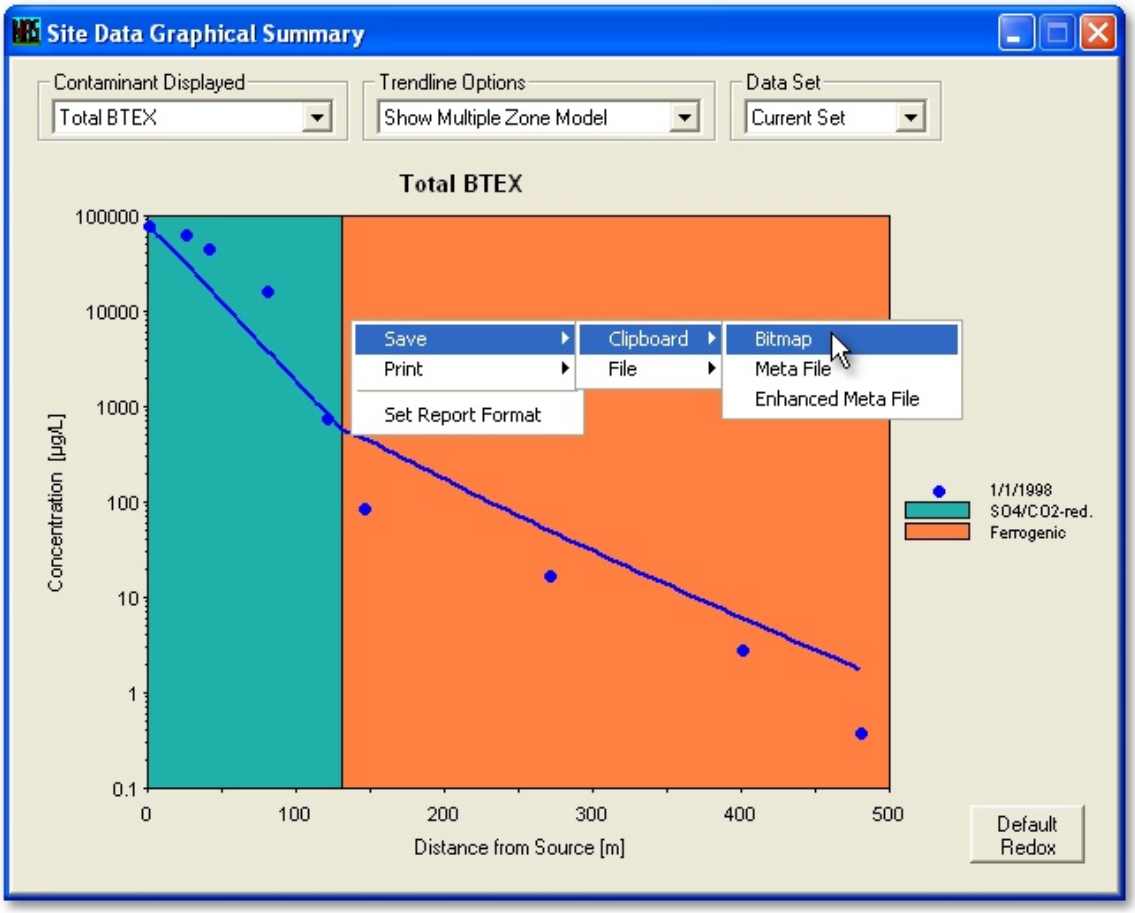


Figure 37. Save/Print PopUp Menu provided for Graphs

APPENDICES

*Appendix A. *.NAS File Structure*

Table 2. *.NAS File Structure

Line	Variable	Format	Description
1	NASVER	None	NAS Version the file was compiled in
2	Blank Line	None	
3	SDINPUT	I5	Flag to indicate completed input for the Site Data Module: =0, General Tab is complete; =1, Hydrogeology Tab is complete; =2, Contaminants Tab is complete; =3, Contaminant Data Tab is complete; =4, Redox Indicator Data Tab is complete
	TOSINPUT	I5	Flag to indicate completed input for the Time of Stabilization Module: =0, POC has been saved; =1, RCCs have been saved
	TORINPUT	F5.0	Flag to indicate completed input for the Time of Remediation Module: =1, Solution Options Tab is complete; =1.4, Solution Options Tab is complete and SCCs have been saved after Simulation Execution; =2, Pump and Treat Tab is complete
4	Descriptive Text	None	*** Site Data Form ***
(Continue if SDTab >= 0)			
5	FACNAME	A50	Facility Name
6	SITENAME	A50	Site Name
7	ADDLDESC	A50	Additional Description
8	LUNIT	A10	Length Unit: 'm' OR 'ft'
	TUNIT	A10	Time Unit: 'd' OR 'yr'
	MUNIT	A10	Mass Unit: 'kg' OR 'lb'
(Continue if SDTab >=1)			
9	KSUBHL	F10.0	Hydraulic Conductivity - Minimum Estimate
	KSUBHB	F10.0	Hydraulic Conductivity - Best Estimate
	KSUBHH	F10.0	Hydraulic Conductivity - Maximum Estimate
10	HYGRADL	F10.0	Hydraulic Gradient - Minimum Estimate
	HYGRADB	F10.0	Hydraulic Gradient - Best Estimate
	HYGRADH	F10.0	Hydraulic Gradient - Maximum Estimate
11	WPOCL	F10.0	Weight Percent Organic Carbon - Minimum Estimate
	WPOCB	F10.0	Weight Percent Organic Carbon - Best Estimate
	WPOCH	F10.0	Weight Percent Organic Carbon - Maximum Estimate

12	TPOR	F10.0	Total Porosity
	EPOR	F10.0	Effective Porosity
	SZ	F10.0	Contaminated Aquifer (Source) Thickness
	SY	F10.0	Source Width
	SX	F10.0	Source Length
13	Descriptive Text	None	*** Contaminant Source ***

(Continue if SDTab >= 2)

14	Descriptive Text	None	*** Headers for Columnar Data ***
15	CGNAME	A50	Contaminant Group Name
16	CGTYPE	I10	Type of Contaminant Group: =0, Non-reactives; =1, Electron donors; =2, Electron acceptors; =3, Co-mingled
	CGNUM	I10	If CGTYPE=3 then CGNUM=Number of Contaminant Groups in Co-Mingled Group, else CGNUM=Number of Contaminants in Group

(if CGTYPE=3 then Enter lines 16-17 CGNUM more times)
(Enter line 17 CGNUM times)

17	CONTNAME	A50	Contaminant Name
	CONTMW	F10.0	Contaminant Molecular Weight
	CONTSOL	F10.0	Contaminant Solubility
	CONTKOC	F10.0	Contaminant Carbon Matter Partition Coefficient
	CONTFRAC	F10.0	Contaminant Initial Mass Fraction in NAPL
	CONTTOT	I10	Contaminant is a Summation of Contaminants Flag: < 0, contaminant represents a summation of individual contaminants; = 0, contaminant is not represented within a total summed contaminant; > 0, contaminant is represented within a total summed contaminant, with the value representing the index of that total contaminant
	CONTCD	I10	Contaminant Concentration Distribution Flag: = 0,the user has not provided a C vs.X profile for the contaminant; = 1, the user has provided a C vs.X profile for the contaminant
	CONTNPL	I10	Contaminant in NAPL Source Flag: = 0, the contaminant is not included in the NAPL source in the TOR simulation; = 1, the contaminant is included in the NAPL source in the TOR simulation
	CONTGC	F10.0	Contaminant Stoichiometric Factor to Daughter: If CGTYPE = 2, then CONTGC represents the stoiciometric factor relating degradation of the electron acceptor to its daughter product
	CONTDF	I10	Contaminant Alternate Pathway Flag: = 0, contaminant does not represent an alternate pathway; < 0, contaminant represents an alternate pathway daughter product, with the absolute value representing the index of the parent contaminant

	CONTDP	F10.0	Contaminant Percent from Parent: If CONTDF < 0, then CONTDP represents the Percent of mass (in aqueous phase concentration) of Parent, reserved for the production of this Daughter product
18	Descriptive Text	None	*** Contaminant and Redox Data ***

(Continue if SDTab >= 3)

19	CONTDS	I10	Number of Contaminant Data Sets
	REDOXDS	I10	Number of Redox Indicator Data Sets

(Enter lines 20-21 CONTDS times)

20	CDSDATE	A10	Date Contaminant Data Set was Sampled (Format: mm/dd/yyyy)
	CDSNUM	I10	Number of Wells in Contaminant Data Set

(Enter line 21 CDSNUM times)

21	CWNAME	A15	Contaminant Well Name
	CWDIST	F15.0	Contaminant Well Distance from Source (First Well must be Source Well, i.e. Distance=0)

(Enter for each CGNUM with CONTCD=1 and CONTTOT>=0)

	CWCONT	F15.0	Contaminant Concentration in Well (ug/L) (NS=Not Sampled, BD=Below Detection)

(Continue if SDTab >= 4)
(Enter line 22-24 REDOXDS times)

22	RDSDATE	A10	Date Redox Indicator Data Set was Sampled (Format: mm/dd/yyyy)
	RDSNUM	I10	Number of Wells in Redox Indicator Data Set
23	RI(8)	8L2	Flags for Redox Indicator Options: Oxygen, Nitrate, Mn(II), Iron(II), Sulfate, Sulfide, Methane, Hydrogen. Enter T to include the option in the simulation, enter F to omit. RI(1), RI(4), RI(5) will always be set to T.

(Enter line 24 RDSNUM times)

24	RWNAME	A15	Redox Well Name
	RWDIST	F15.0	Redox Well Distance from Source

(Enter for each RI()=T)

	RWCONT	F15.0	Redox Concentration in Well (mg/L, if Hydrogen then nM) (NS=Not Sampled, BD=Below Detection)
25	Descriptive Text	None	*** TOS/DOS Form ***

(Continue if TOSTab >= 0)

26	POC	F10.0	Distance from Source to Point of Compliance
	TOSDATE	A10	Date Source Reduction was accomplished (Format: mm/dd/yyyy)

(Continue if TOSTab >= 1)
(In line 27, enter for each CGNUM with CONTCD=1)

27	RCC()	()F10.0	Regulatory Compliance Concentration at the Point of Compliance (ug/L)
28	Descriptive Text	None	*** TOR Form ***

(Continue if TORTab >= 1)

29	NPLOPT	I5	NAPL Mass estimate option:Enter 0 for Best Estimate only; Enter 1for Best, Maximum, and Minimum Estimates;Enter 2 for Best Estimate, and Percent(+/-) of Best Estimate
	REMOPT	I5	NAPL Source removal option: Enter 0 for no Mass Removal; Enter 1-3, for 1 to 3 different Mass Removal Plans
	TORDATE	A10	Date Source Emplaced or Reduction was accomplished (Format: mm/dd/yyyy)
30	NPLMASS()	()F10.0	Estimated NAPL Mass: If NPLOPT=0-Enter Best Estimate;If NPLOPT=1-Enter Best, Maximum, and Minimum Estimates;If NPLOPT=2-Enter Best Estimate, and Percent(+/-) of Best Estimate

(Enter line 31 if REMOPT>0)

31	NPLREM()	()F10.0	Source Removal Plans: Enter Percent(%) Removal REMOPT times
32	PERLEN	F10.0	Maximum length of TOR simulation time, in years
	VELRNG	L10	Flag to simulate range in velocities: Enter F to simulate Best Estimate velocity only; Enter T to simulate Minimum, Best Estimate, and Maximum velocities

(Continue if TORTab >= 1.4)
(In line 33, enter for each CGNUM with CONTCD=1 or CONTNPL=1)

33	SCC()	()F10.0	Compliance Concentration at the Source (ug/L)

(Continue if TORTab >= 2)

34	PTMOD	L2	Pump and Treat flag: Enter T to simulate Pump and Treat to compare with MNA; Enter F to not simulate MNA only

(Enter if PTMOD=T)

	PTAVSAT	F10.0	Average saturated thickness of aquifer

(Enter lines 35-36 if PTMOD=T)

35	PTOPT(3)	3L2	Pump and Treat Flags: PTOPT(1)-Flag for Pumping Well Distance from source; PTOPT(2)-Flag for Pumping Well Rate (<=PERLEN); PTOPT(3)-Flag for Pumping Well Duration. Enter T if parameter will be specified by user, enter F if parameter will be estimated by NAS.

(In line 36, enter for each PTOPT()=T)

36	PTUSER()	()F10.0	User-specified Pump and Treat parameters.

(Lines 37-40 always printed)

37	Descriptive Text	None	*** Data/Results Output Format ***
38	FRMEXP	A100	Page formatting for print/saved form of the 'Data and Results Table'
39	FRMHEAD	A100	Text and format of headers on printed/saved form of the 'Data and Results Table'
40	FRMFOOT	A100	Text and format of footers on printed/saved form of the 'Data and Results Table'

Appendix B. NAS Contaminant Database File Structure

Table 3. NAS Contaminant Database File Structure

Line	Row	Col	Variable	Description
1	1	A	Descriptive Text	*** Number of Groups ***
2	1	B	NUMCGS	Number of Contaminant Groups in Database
	2		Descriptive Text	*** Headers for Columnar Data ***
(Enter lines 3-6 NUMCGS times)				
3	+1		Blank Line	
4	+1	A	CGNAME	Contaminant Group Name
5	+1	B	CGTYPE	Type of Contaminant Group: = "Non-reactive" ; = "Electron Donors" ; = "Electron Acceptors" ; = "Co-mingled"
		D	CGNUM	If CGTYPE="Co-mingled" then CGNUM=Number of Contaminant Groups in Co-Mingled Group, else CGNUM=Number of Contaminants in Group
(if CGTYPE="Co-mingled" then Enter lines 3-6 CGNUM more times)				
(Enter line 6, CGNUM times)				
6	+1	A	CONTNAME	Contaminant Name
		B	CONTMW	Contaminant Molecular Weight
		C	CONTSOL	Contaminant Solubility
		D	CONTKOC	Contaminant Carbon Matter Partition Coefficient
		E	CONTFRAC	Contaminant Initial Mass Fraction in NAPL
		F	CONTTOT	Contaminant is a Summation of Contaminants Flag: < 0, contaminant represents a summation of individual contaminants; = 0, contaminant is not represented within a total summed contaminant; > 0, contaminant is represented within a total summed contaminant, with the value representing the index of that total contaminant
		G	CONTCD	Contaminant Concentration Distribution Flag: = 0,the user has not provided a C vs.X profile for the contaminant; = 1, the user has provided a C vs.X profile for the contaminant
		H	CONTNPL	Contaminant in NAPL Source Flag: = 0, the contaminant is not included in the NAPL source in the TOR simulation; = 1, the contaminant is included in the NAPL source in the TOR simulation
		I	CONTGC	Contaminant Stoichiometric Factor to Daughter: If CGTYPE = 2, then CONTGC represents the stoiciometric factor relating degradation of the electron acceptor to its daughter product

J	CONTDF	Contaminant Alternate Pathway Flag: = 0, contaminant does not represent an alternate pathway; < 0, contaminant represents an alternate pathway daughter product, with the absolute value representing the index of the parent contaminant
K	CONTDP	Contaminant Percent from Parent: If CONTDF < 0, then CONTDP represents the Percent of mass (in aqueous phase concentration) of Parent, reserved for the production of this Daughter product

Appendix C. Determining Redox Conditions

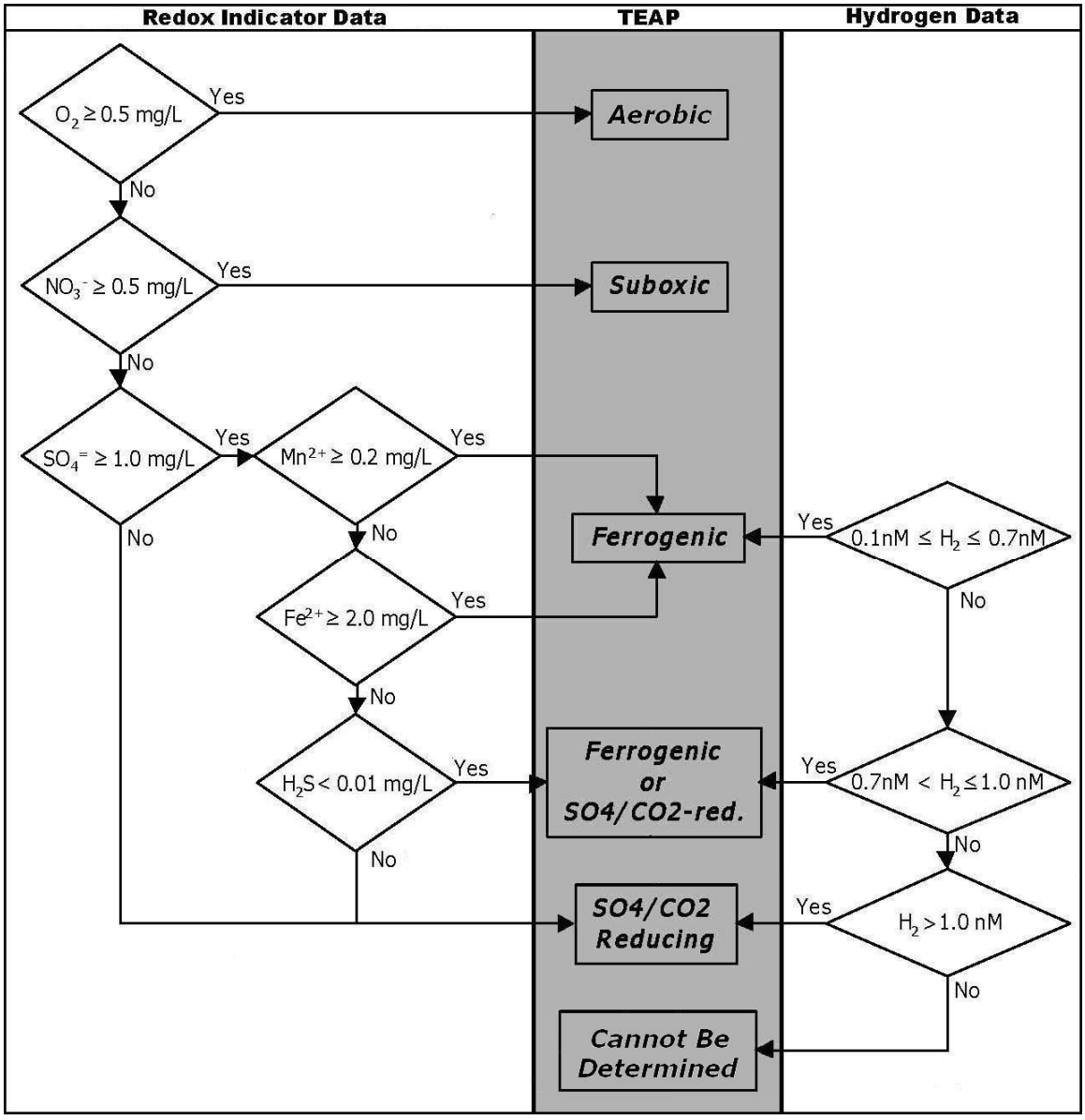


Figure 38. Flow Chart for Determining Redox Conditions