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rtFlux: RT3D Flux Plane Utility

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M. J. Truex

July 2006

Prepared for
Groundwater Services, Inc.
Houston, Texas 77098
under Contract 48146

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Summary

A flux plane software utility called rtFlux was developed as a *Microsoft*® *Excel*®-based pre- and post-processor for a RT3D simulation. The rtFlux utility provides a method for the user to determine the mass flow of chemical species across one or more grid-orthogonal planes over time. Mass flow results are presented as time series plots and as plots showing the spatial distribution of the relative mass flow within a given plane. This document discusses how to install and use the rtFlux software, the calculations that are performed, and gives some examples of the application of the rtFlux utility.

Acknowledgment

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1.0 Introduction

Monitored natural attenuation (MNA) is an environmental management strategy that relies on a variety of attenuation processes to degrade or immobilize contaminants and is implemented at appropriate sites by demonstrating that contaminant plumes have low risk and are either stable or shrinking. Numerical modelling can be one component of an assessment of MNA or Enhanced Attenuation (EA) (i.e., if MNA is not a viable single remedy). Numerical reactive transport modelling provides a tool with which to quantify the relative stability of a contaminant plume, particularly in cases where simpler evaluations are not suitable because of complex hydrology, past activity at the site, multiple contaminant sources, and/or complex reaction of multiple species. Selection of an appropriate model configuration to represent spatial and temporal variations in site-specific attenuation processes can facilitate assessment of the contaminant loading and attenuation capacity (i.e., mass balance) at the site.

RT3D is a numerical code for simulating three-dimensional multi-species reactive transport in groundwater [Clement, 1997; Clement et al., 1998; Clement and Johnson, 2002; Johnson et al., 2006a]. RT3D can provide information to help analyze the relative importance of different fate and transport processes at an individual site and assess the plume in terms of a mass balance approach. The model can also be used to estimate the future fate and transport of contaminants. These predictions can be valuable input, along with other site information, in making timely decisions regarding implementation of remedial actions or for planning monitoring activities. A key function of the predictive capability of models is to estimate whether the remedy will meet the remediation goals when this determination cannot be made directly with field data.

The typical output from numerical modelling is the spatial distribution of contaminant concentration as time progresses. Such concentration information is the primary metric in determining the success of a remediation scenario with respect to the goal of protecting receptors. However, the mass flux (flow) across a specified plane can provide additional information for making remediation decisions. Mass flux can be a useful indicator of the potential for MNA. Evaluation of the temporal changes in mass flux can reveal the nature of plume migration (expanding, steady state, shrinking) and the time frame to reach a steady state. The mass flux can also be used in quantifying contaminant plume dynamics and the impact of treatment processes. The mass flux from a contamination source defines the amount of attenuation (natural or otherwise) that will be required for a remedy protective of the receptors.

A flux plane software utility called rtFlux was developed as a *Microsoft® Excel®*-based pre- and post-processor for a RT3D simulation. The rtFlux utility provides a method for the user to determine the mass flow of chemical species across one or more grid-orthogonal planes over time. Mass flow results are presented as time series plots and as plots showing the spatial distribution of the relative mass flow terms for a given plane.

Flux planes of interest are defined as rectangular regions that are orthogonal to the model grid (i.e., the plane is aligned parallel to a row, column, or layer of the model grid). The pre-processing step incorporates the flux plane definitions into the RT3D input files. After running RT3D, the output files are processed by the utility to generate three graphs that describe the mass flux across the plane. The first plot shows the time-varying mass flow rate (e.g., kg/day) of each chemical species passing through one of the defined planes. The second plot depicts the cumulative mass that has passed through a plane over time. The underlying data for this plot can be interrogated to obtain a table listing the mass passing through the plane during a specified time interval. The third plot generated from the rtFlux utility is a bubble plot depicting the relative volumetric flow rate, species concentration, or mass flow rate through a plane at each grid cell in a plane. This bubble plot shows the location where the highest mass flux impacts occur, whether due to high volumetric flow rate or a high concentration (or combination of both).

This document discusses how to install and use the rtFlux software, the calculations that are performed, and gives some examples of the application of the rtFlux utility.

2.0 Installation of rtFlux

The rtFlux utility is implemented in two key pieces – a processing engine and a user interface. The processing engine is an executable file that does the behind-the-scenes work of modifying the RT3D input files and processing results. The user interface portion of the rtFlux utility is provided as a *Microsoft®* *Excel®* template workbook (*.xlt) and is where the user interaction takes place.

2.1 System Requirements

The following hardware and software are required to use the rtFlux utility:

- *IBM®*-compatible personal computer with an *Intel®* *Pentium®*-compatible processor or greater,
- Monitor resolution of at least 1152 × 864 pixels
- *Microsoft®* *Windows®* 2000 or *Microsoft®* *Windows®* XP operating system,
- *Microsoft®* *Excel®* 2000 or *Microsoft®* *Excel®* 2003,
- RT3D version 2.5 or greater
- MODFLOW (any version compatible with RT3D)

2.2 Installation

To make the rtFlux interface available in *Microsoft®* *Excel®*, the template file must be placed (or saved) into the "Templates" directory. The "Templates" directory is typically found in the directory tree at "C:\Documents and Settings\<username>\Application Data\Microsoft\Templates" for recent versions of *Microsoft®* *Windows®*, where <username> is the actual user name of the current *Windows®* user. A hard drive search may be helpful in determining the actual location of the "Templates" directory.

The processing engine (rtFlux.exe) must be placed in a directory that is in the *Windows®* system search path (defined by the %PATH% environment variable – see your *Windows®* documentation for information on editing environment variables).

2.3 Uninstalling the rtFlux Utility

To uninstall the rtFlux utility, remove (move or delete) the rtFlux template file from the "Templates" directory. This will remove it from the list of document templates in the File/New… dialog box. Removal of the rtFlux.exe file from the directory where you originally placed it will complete the uninstallation.

2.4 Updating to a New Version

Each version of the rtFlux template file will have a unique filename to identify the version of the template (e.g., "rtFlux_1_0_0.xlt"). To update to a newer version, the new template file is placed into the "Templates" directory. If desired, the old template file may be removed from the "Templates" directory. New versions of the processing engine will have the same name as the old version and should directly replace the old version.

3.0 Using the rtFlux Utility

The rtFlux software utility is both a pre-processor and post-processor for a RT3D simulation. The user is assumed to be familiar with both MODFLOW [McDonald and Harbaugh, 1988; Harbaugh et al., 2000; Zheng et al. 2001; Harbaugh, 2005] and RT3D [Clement, 1997; Clement et al., 1998; Clement and Johnson, 2002; Johnson et al., 2006a] as well as the process of defining a model, running the numerical codes, and accessing the resultant output. While MODFLOW and RT3D models are often configured and run from within a third party graphical user interface such as GMS [BYU, 2006], Visual Modflow [WHI, 2005], PMWIN [Chiang, 2005], or Groundwater Vistas [Rumbaugh and Rumbaugh, 2004], the rtFlux software runs external to these groundwater modelling software packages.

The following list summarizes the steps for using the rtFlux utility with an RT3D simulation. Subsequent subsections describe specific actions and the rtFlux toolbar in more detail.

- Configure the MODFLOW model for the site and run MODFLOW. The MODFLOW model must use the LKMT Package [Zheng et al., 2001].
- Configure the RT3D model for the site and save/export the configuration to the RT3D input files.
- In *Excel*®, create a new rtFlux workbook by selecting the File/New… menu item and opening the rtFlux template file as a new workbook.
- Add data to the "rtFlux_Input" worksheet to define the basic model configuration and the locations for flux planes.
- Export the plane definitions. This will modify the RT3D *.btn input file; any existing observation points in the *.btn file will be deleted. Note that if the RT3D input files are saved/exported from a groundwater modelling software package, the exported plane definitions will be lost.
- Run RT3D. This may be done from within *Excel*®, from within a groundwater modelling software package (as long as files aren't saved/exported as part of the run command), or from the command prompt (DOS window).
- In *Excel*®, initiate the action to process the RT3D simulation results and import the flux plane data into the rtFlux workbook. Depending on the size of the model, it may take a while to process the RT3D simulation results. Once the flux information is imported, the user may assess the results displayed on the "Graphs" worksheet.

3.1 Creating a rtFlux Workbook

To generate a new rtFlux workbook, the rtFlux template file is opened from the File/New… menu item. This will create an empty, unsaved document with all of the necessary functionality and will make an "rtFlux" toolbar available. The new document can be saved and subsequently opened in the same manner as any other *Microsoft*® *Excel*® workbook.

3.2 Saving and Opening a rtFlux Workbook

When first created, a rtFlux workbook is not automatically saved, so the user will need to save the file. When creating or re-opening a rtFlux workbook, the user may receive a message that the workbook contains macros. There are several macros in the rtFlux workbook that are required for calculations to work properly, thus the user should select the "Enable Macros" option. Newer versions of *Microsoft® Excel®* have additional security options found under the Tools/Macro/Security… menu item. If "High Security" is selected, then all macros are disabled by default (with no user prompting) and the rtFlux workbook will not operate correctly. The user should check the security settings and change to "Medium Security" to allow the user to confirm, on an individual workbook basis, whether macros should be enabled or not.

If the user opens a rtFlux workbook with macros disabled, a non-functional rtFlux toolbar will appear. This non-functional rtFlux toolbar must be removed manually from the *Microsoft® Excel®* workspace before the user can once again use a rtFlux workbook properly. To remove the toolbar, close all open rtFlux workbooks and delete the toolbar from the toolbar list shown in the "Customize" dialog box (opened by right clicking on any toolbar and selecting "Customize" or via the Tools/Customize… menu item).

3.3 Description of the rtFlux Toolbar Items

Whenever a rtFlux workbook is created or opened, the "rtFlux" toolbar will appear in the *Microsoft® Excel®* workspace. When the last rtFlux workbook is closed, the rtFlux toolbar will disappear. Figure 1 shows the rtFlux toolbar and the toolbar button functionality is described in Table 1. To insure integrity of the rtFlux utility, **do not** alter the rtFlux toolbar by adding or removing buttons via the Tools/Customize… menu item. Modification of the rtFlux toolbar may cause the associated functions to fail.

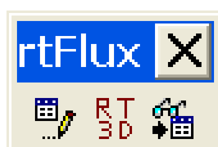

Figure 1. *Toolbar for the rtFlux Utility — From left to right the toolbar buttons are: Modify the BTN File to Incorporate Flux Plane Definition(s), Run RT3D, and Process Flux Output and Read Into Excel.*

Table 1. *Functionality of the rtFlux Toolbar Buttons*

Button	Description
Export Plane Definitions 	This button activates a procedure that examines the plane definitions for validity, exports the plane definitions to a *.iob file, and runs the rtFlux engine to incorporate the plane definitions into the *.btn file for the simulation.
Run RT3D 	This button initiates a RT3D simulation run. MODFLOW should have been previously run. RT3D will run for valid model input files regardless of whether flux plane definitions have been exported or not.
Import Results 	This button will start the rtFlux engine to process the RT3D simulation output and generate the flux data; this step may take a while to complete depending on the size of the model. Once the flux data is generated, it is read into the workbook and the plots are set up.

3.4 Defining and Exporting Flux Plane Definitions

To obtain the mass flow through a plane over time from a RT3D simulation, the user must define the flux planes of interest on the "rtFlux_Input" worksheet (Figure 2). Light blue cells on the "rtFlux_Input" worksheet indicate the information to be supplied by the user. Basic information about the model (number of rows, columns, and layers) and the number of flux planes that will be defined are the first items to fill in. The flux planes must be defined as orthogonal to the grid—that is, each plane must be parallel to a row, column, or layer. Flux planes are defined as a rectangular area by specifying the grid cell indices of opposing corners. In effect, this defines the starting and ending rows, columns, and layers for the plane. The standard convention of cell index numbers is used, where the numbers increase from the upper left cell of the top layer (in plan view) to the right (for columns), to the bottom (for rows), and down (for layers). If the plane definition is ambiguous as to the orientation, the user must specify the type of plane (i.e, XY, XZ, or YZ). Each plane is assigned a group identification number automatically, which should not be modified by the user. The Plane Identifier data entry field allows the user to annotate each plane with a name or brief description, but is not actually used elsewhere. Units used in the simulation need not be specified to export the plane definitions, but they are required for importing results.

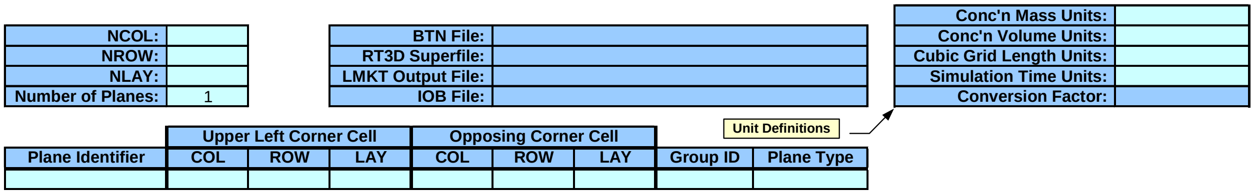

Figure 2. *The rtFlux Plane Definitions Are Specified Using This Data Entry Layout on the "rtFlux_Input" Worksheet — The lighter blue shading indicates information that must be filled out by the user. The lower block expands to accommodate the number of planes that the user wants to define.*

Once defined, plane definitions can be exported to an existing RT3D simulation using the "Export Plane Definitions" button on the rtFlux toolbar. In the export process, the plane definitions are validated, exported to an *.iob file, and then incorporated into the *.btn RT3D input file via the rtFlux engine. This process takes place automatically aside from the user specifying the location and names for the *.iob file and the *.btn file (which should both be in the same directory). When plane definitions are exported, any existing observation points in the *.btn file will be deleted. Note that if the RT3D input files are saved/exported from a groundwater modelling software package, the exported plane definitions will be lost.

Because the *.iob file is generated automatically, the user will merely need to know that the file is created and that it needs to be saved to the same directory containing the RT3D simulation input files. However, for completeness, the structure of the ASCII text *.iob file is described in Table 2.

Table 2. *File Structure for the *.iob File, Containing Flux Plane Definitions*

Record	Conditions for Record	Field(s)	Field Description(s)	Format
H1	—	NPLANE	number of planes defined	I10
H2	Repeat this record NPLANE times.	COLS COLE ROWS ROWE LAYS LAYE GRP PTYPE	Starting column of plane Ending column of plane Starting row of plane Ending row of plane Starting layer of plane Ending layer of plane Group ID number for this plane Plane type (XY, XZ, YZ) ID number	7I10

Once the flux plane definitions are successfully exported, RT3D may be executed by the most convenient method. The RT3D executable file must be in a directory that is in the system search path to run RT3D via the rtFlux toolbar button in *Excel*®. RT3D may be run from within a groundwater modelling software package as long as the run command does not save/export the RT3D input files. More advanced users may prefer to run RT3D from s command prompt (DOS window). Note that data for the flux plane utility is recorded for every transport step, meaning that the RT3D output files (*.obs) may be large for long or complex simulations.

3.5 Processing and Viewing Flux Plane Results

After running RT3D to produce simulation results, the results can be processed and flux information imported to the rtFlux workbook. The Import Results button on the rtFlux toolbar activates the rtFlux engine to process the RT3D output and generate flux-related data. This step may take a while, depending on the size of the RT3D model (in terms of grid size, number of chemical species, and total simulated time). The user must specify the LKMT output file from the MODFLOW simulation (e.g., *.hff, *.flo) and confirm the *.btn file to use.

Data for the flux planes are imported to tables on a number of worksheets (see Table 3). The "Graphs" worksheet is of primary interest to the user, as it contains the compiled data in three plots and a summary table. The first plot (Figure 1) shows the time-varying mass flow rate (e.g., kg/day) of chemical species at the defined planes. The user may select the chemical species and/or flux plane to display from a drop-down list at the worksheet cells in light blue. The direction of net mass flow is determined by knowing the type of plane (XY, XZ, or YZ) and whether the values are positive (flow in the +x, -y, or -z direction) or negative (flow in the -x, +y, or +z direction). The plot of cumulative mass passing through a plane over time has options similar to those for the mass flow plot.

Table 3. *List of Worksheets in a rtFlux Workbook*

Worksheet	Information Contained on Worksheet
rtFlux_Input	Flux Plane Definitions
Graphs	Graphs & Tables of Flux Utility Results
Mass_Flow_Data	Data for the Mass Flow Plot
Cumulative_Mass_Data	Data for the Cumulative Mass Plot
Cell_Data	Data for the Bubble Plot
Cumulative_Mass_Positive_Direct	Data for the Cumulative Mass Table
Cumulative_Mass_Negative_Direct	Data for the Cumulative Mass Table

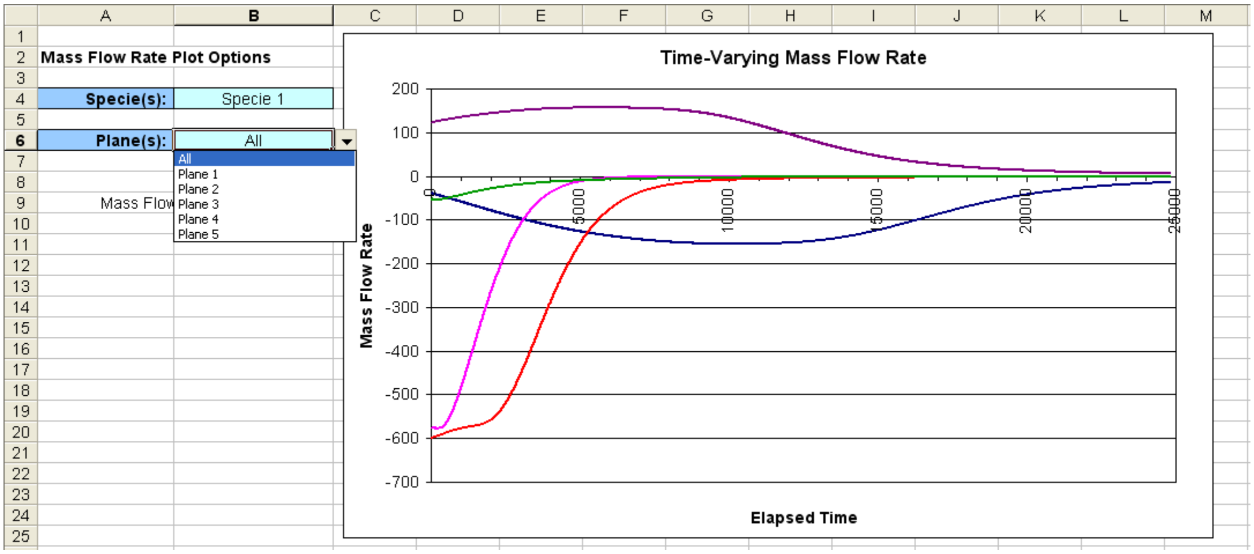

Figure 3. *The Time-Varying Mass Flow Rate Plot on the "Graphs" Worksheet — The user may select which species and which plane to view (including all at once) via drop-down selection lists. The cumulative mass flowing through the plane plot is also on the "Graphs" worksheet and is configured similarly.*

Figure 4 shows an example of the third plot generated by the rtFlux utility. This bubble plot depicts the relative volumetric flow rate, species concentration, or mass flow rate through a plane at each grid cell in a plane. The user may select the parameter, the species, the plane, and the simulation time to display in the bubble plot. Because *Excel*® is limited in the number of rows of data that may be imported, not all transport time points may be imported. The rtFlux utility imports cell-by-cell data for the bubble plot at regularly spaced time points, the frequency of which depends on the total number of grid cells in all the planes and the total number of transport time points. The bubble plot shows the spatial distribution within the plane where the highest mass flux impacts occur. The highest mass flow may be due to a high volumetric flow rate, a high concentration, or a combination of both. The bubbles represent the relative magnitude of the displayed parameter and are scaled relative to the maximum of the entire dataset so changing to a different time point will show the proper relative change in parameter values. The user should be aware that the scaling might cause bubbles for low parameter values to disappear because the relative magnitude is so small. The graph properties can be modified by the user to make small values visible as bubbles at the expense of causing large bubbles to overlap. The bubble plots show the distribution of parameter values in the plane for a uniformly spaced grid. Non-uniform grids or deformed grids will be displayed within a uniform grid.

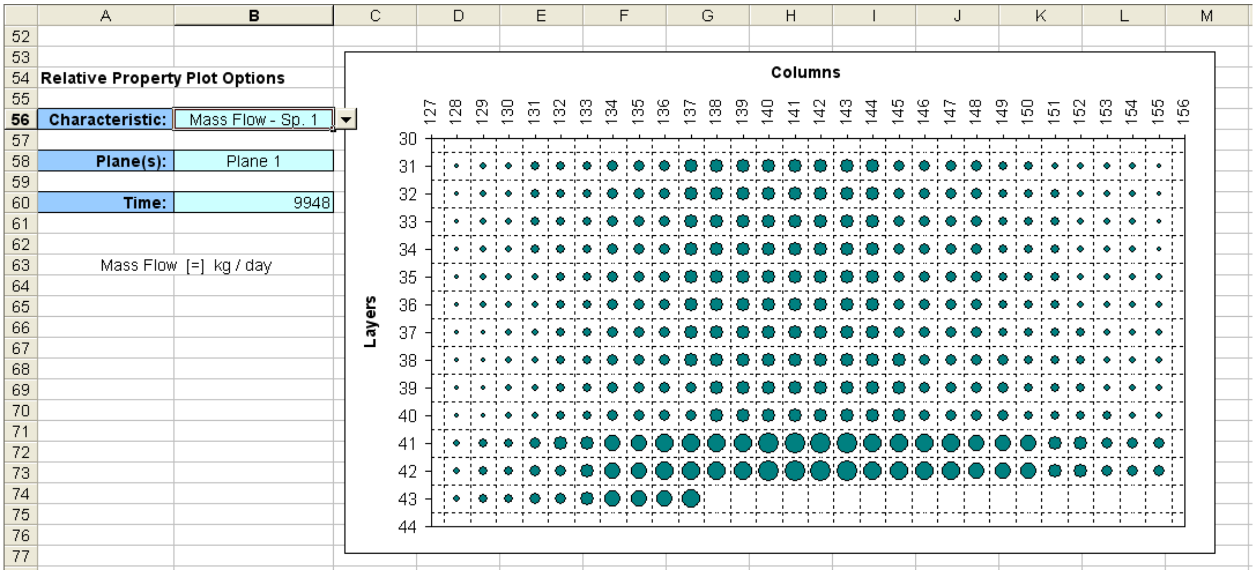

Figure 4. *Example of a Bubble Plot Showing the Relative Magnitude of Mass Flow Rate for a Specified Plane at a Particular Time Point in the Simulation — Drop down lists allow the user to select the property (also including volumetric flowrate and concentration), plane, and time to display. The bubble sizes are scaled relative to the largest value in the simulation so that the size shows the proper relative magnitude when looking at different time points.*

A summary table of cumulative mass passing through each plane for each species is included at the bottom of the "Graphs" worksheet. This table shows the mass moving in both positive (+x, -y, or -z) and negative (-x, +y, or +z) directions as well as the net cumulative mass passing through each plane (which is what is plotted in the cumulative mass plot). Mass may flow in both directions through a plane depending on the steady state or transient flow characteristics at the location where the plane is defined. Start and end times at points within the time frame of the simulation may be selected via drop-down lists to view the cumulative mass for a specified period. An example of this summary table is shown in Figure 5.

Begin Time:	0
End Time:	24820

Cumulative Mass Flowing Through Plane				
Specie #	**Plane #**	**Total Mass Thru Plane in Positive Direction (kg)**	**Total Mass Thru Plane in Negative Direction (kg)**	**Net Mass Thru Plane (kg)**
1	1	2091799	-0.353	2091799
1	2	15143.47	-2422723	-2407580
1	3	3.08163	-1210683	-1210680
1	4	743.8011	-2517156	-2516413
1	5	52427.44	-226410	-173983

Figure 5. *Example of the Summary Table for Cumulative Mass Flowing Through Each Plane on the "Graphs" Worksheet — This table shows the mass moving in both positive (+x, -y, or -z) and negative (-x, +y, or +z) directions as well as the net cumulative mass passing through each plane. The user may select the start and end times to apply to the table to view the cumulative mass for a specified period.*

The remaining worksheets in the rtFlux workbook (Table 3) contain the root data on which the plots and summary table are based. Figures 6 to 8 show partial examples of data on the "Mass_Flow_Data," "Cumulative_Mass_Data," and "Cell_Data" worksheets, respectively. The "Cumulative_Mass_Positive_Direct" and "Cumulative_Mass_Negative_Direct" worksheets are configured the same as the "Cumulative_Mass_Data" worksheet, but contain cumulative mass moving in the positive and negative directions, respectively, instead of the net mass passing through the plane. The user will not typically need to interact with these worksheets. However, the "Cell_Data" worksheet is configured to allow data filtering to make interrogation of the cell-by-cell data set more convenient. Note that filtering of the cell-by-cell data will impact what is displayed in the bubble plot.

Number of Time Steps:	2505
Number of Planes:	5
Number of Species:	1

MASS FLOW RATE

(kg / day)

	Plane # 1 Specie # 1	Plane # 2 Specie # 1	Plane # 3 Specie # 1	Plane # 4 Specie # 1	Plane # 5 Specie # 1
Elapsed Time	Sp 1, P 1	Sp 1, P 2	Sp 1, P 3	Sp 1, P 4	Sp 1, P 5
0.1	123.308	-38.4394	-575.82	-598.777	-50.8043
10.1	123.4393	-38.6626	-575.909	-598.461	-51.507
20.1	123.5704	-38.8823	-575.987	-598.186	-52.0471
30.1	123.7011	-39.0995	-576.057	-597.931	-52.472
40.1	123.8316	-39.3148	-576.126	-597.695	-52.8111
50.1	123.9617	-39.5284	-576.192	-597.463	-53.0864
60.1	124.0917	-39.7405	-576.258	-597.24	-53.3122
70.1	124.2211	-39.9513	-576.323	-597.018	-53.4991
80.1	124.3503	-40.1609	-576.39	-596.799	-53.6538
90.1	124.4791	-40.3693	-576.457	-596.581	-53.7818
100.1	124.6076	-40.5767	-576.524	-596.363	-53.8861
110.1	124.7361	-40.7832	-576.591	-596.144	-53.9704
120.1	124.8642	-40.9888	-576.657	-595.924	-54.0365

Figure 6. *Partial Example of the "Mass_Flow_Data" Worksheet, Where Data for the Mass Flow Rate is Stored*

NET CUMULATIVE MASS

(kg)

	Plane # 1 Specie # 1	Plane # 2 Specie # 1	Plane # 3 Specie # 1	Plane # 4 Specie # 1	Plane # 5 Specie # 1
Elapsed Time	Sp 1, P 1	Sp 1, P 2	Sp 1, P 3	Sp 1, P 4	Sp 1, P 5
0.1	6.165401	-1.92197	-28.791	-29.9388	-2.54022
10.1	1239.902	-387.432	-5787.43	-6016.13	-514.097
20.1	2474.951	-775.157	-11546.9	-11999.4	-1031.87
30.1	3711.308	-1165.07	-17307.1	-17979.9	-1554.46
40.1	4948.971	-1557.14	-23068	-23958.1	-2080.88
50.1	6187.938	-1951.35	-28829.6	-29933.9	-2610.37
60.1	7428.205	-2347.7	-34591.9	-35907.4	-3142.36
70.1	8669.769	-2746.16	-40354.8	-41878.7	-3676.42
80.1	9912.626	-3146.72	-46118.4	-47847.7	-4212.18
90.1	11156.77	-3549.37	-51882.6	-53814.6	-4749.36
100.1	12402.21	-3954.1	-57647.5	-59779.4	-5287.7
110.1	13648.93	-4360.9	-63413.1	-65741.9	-5826.98
120.1	14896.93	-4769.76	-69179.3	-71702.2	-6367.02

Figure 7. *Partial Example of the "Cumulative_Mass_Data" Worksheet Holding the Data for Net Cumulative Mass Passing Through the Plane*

NOBS:	5082

CELL-BY-CELL DATA

Flow [=] ft³ / day
Conc'n [=] mg / L
Mass Flow [=] kg / day

							Concentration	Mass Flow
Elapsed Time	Plane #	Flow Directi	K	I	J	Volumetric Flow	Specie # 1	Specie # 1
0.1	1	2	27	137	123	0.07677077	0.000263013	5.72E-10
0.1	1	2	27	137	124	0.08001004	0.000266013	6.03E-10
0.1	1	2	27	137	125	0.08311607	0.000279014	6.57E-10
0.1	1	2	27	137	126	0.08608488	0.000310019	7.56E-10
0.1	1	2	27	137	127	0.08891378	0.00290927	7.32E-09
0.1	1	2	27	137	128	0.09160565	0.00889974	2.31E-08
0.1	1	2	27	137	129	0.0941678	0.0174664	4.66E-08
0.1	1	2	27	137	130	0.09660601	0.0316423	8.66E-08
0.1	1	2	27	137	131	0.09892444	0.0534557	1.5E-07
0.1	1	2	27	137	132	0.10112538	0.0848855	2.43E-07
0.1	1	2	27	137	133	0.10320929	0.12765	3.73E-07
0.1	1	2	27	137	134	0.10517428	0.18258	5.44E-07
0.1	1	2	27	137	135	0.10701541	0.24997	7.57E-07
0.1	1	2	27	137	136	0.10872402	0.32865	1.01E-06
0.1	1	2	27	137	137	0.11028744	0.4167	1.3E-06
0.1	1	2	27	137	138	0.11168924	0.51103	1.62E-06
0.1	1	2	27	137	139	0.11290935	0.60804	1.94E-06

Figure 8. *Partial Example of the "Cell_Data" Worksheet — This information is used for the bubble plots of volumetric flowrate, concentration, and mass flow rate on an individual cell basis for a given plane.*

4.0 Calculation of Flux Plane Results

The RT3D flux plane utility software performs calculations on concentrations and volumetric flow rates to obtain the net mass flows (e.g., kg/day) through a plane. The term mass flux or flux plane is often mentioned, but differs from a mass flow in that a mass flux is a rate per unit area (e.g., kg/day/m^2). The current version of the rtFlux utility only provides mass flow results, but the user can manually convert mass flow to mass flux based on the area of the "flux plane" (or cross sectional area of individual cells if such resolution is desired). Equations are presented in this section for mass flow, mass flux, and the cumulative mass passing through a plane.

Equations 1 and 2 describe the mass flow and mass flux, respectively, for the portion of a plane that intersects a single grid cell. Generic units are shown using mass (M), length (L), and time (T). The total mass to pass through the cross sectional area of a single grid cell for an incremental time is calculated as the average mass flow rate times the time period (Equation 3).

$$\text{Mass Flow Rate for the p}^{\text{th}}\text{ grid cell } = \dot{m}_{t,p} = C_{t,p} \cdot Q_{i,t,p} \qquad [=]\ \frac{\text{M}}{\text{T}} \tag{1}$$

$$\text{Mass Flux for the p}^{\text{th}}\text{ grid cell } = J_{t,p} = \frac{\dot{m}_{t,p}}{A_{CS,p}} \qquad [=]\ \frac{\text{M}}{\text{T} \cdot \text{L}^2} \tag{2}$$

$$\begin{array}{l}\text{Incremental Mass Passing Through} \\ \quad \text{the Plane in the p}^{\text{th}}\text{ Grid Cell} \\ \quad \text{Over an Incremental Time}\end{array} = \Delta m_{t,p} = \tfrac{1}{2} \cdot \left(\dot{m}_{t,p} - \dot{m}_{t-1,p}\right) \cdot \left(T_t - T_{t-1}\right) \qquad [=]\ \text{M} \tag{3}$$

In these equations, $C_{t,\,p}$ is the concentration at the tth transport time step for the pth grid cell, $Q_{i,\,t,\,p}$ is the volumetric flow rate of the groundwater along the ith axis (X, Y, or Z – whichever is of interest) at the tth transport time step for the pth grid cell, $A_{CS,\,p}$ is the (saturated) cross sectional area for the pth grid cell, and T_t is the elapsed time at the tth transport time step. These equations apply to a single cell based on the concentrations, volumetric flow rates, and cross sectional areas at the cell center. The concentrations are output from the RT3D simulation and the volumetric flow rates are read from the MODFLOW LKMT Package output file.

Equations 4 to 6 provide overall/average values for an entire plane comprised of N_{cell} grid cells having a total cross sectional area of $A_{CS,\,plane}$. Figure 9 depicts the combination of volumetric flow (arrow size) and concentration (color of the boxes) to determine mass flow (thickness of the boxes) for several grid cells and how this information is averaged to produce the result for a plane.

$$\text{Total Mass Flow Rate for Plane } = \dot{m}_{plane,t} = \sum_{p=1}^{N_{cell}} \dot{m}_{t,p} \qquad [=] \quad \frac{\text{M}}{\text{T}} \tag{4}$$

$$\text{Average Mass Flux for Plane } = J_{plane,t} = \frac{\dot{m}_{plane,t}}{A_{CS,\,plane}} \qquad [=] \quad \frac{\text{M}}{\text{T} \cdot \text{L}^2} \tag{5}$$

$$\begin{array}{c}\text{Incremental Mass Passing}\\ \text{Through the Plane}\\ \text{Over an Incremental Time}\end{array} = \Delta m_t = \tfrac{1}{2} \cdot \left(\dot{m}_{plane,t} - \dot{m}_{plane,t-1}\right) \cdot \left(T_t - T_{t-1}\right) \qquad [=] \quad \text{M} \tag{6}$$

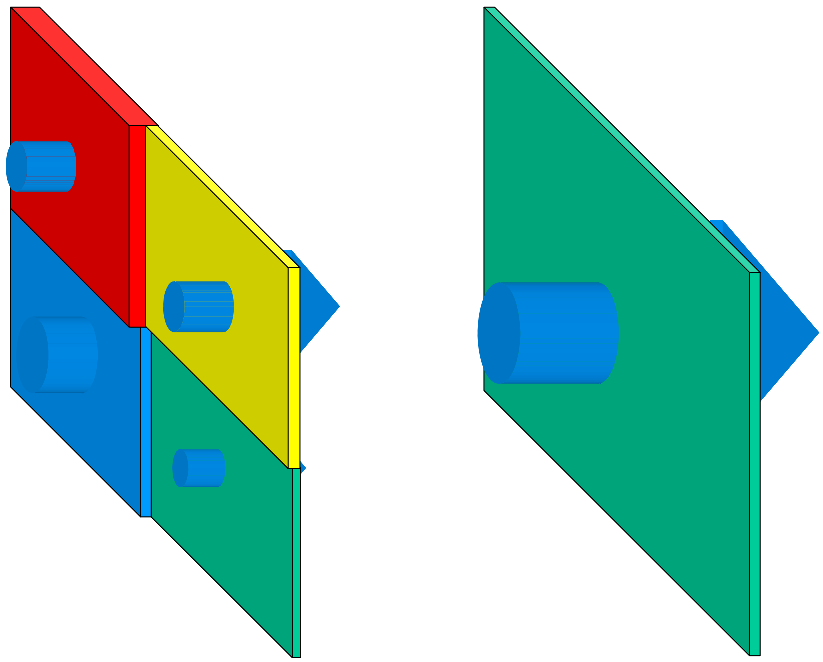

Figure 9. *Depiction of Mass Flow Through the Grid Cells That Comprise an Entire Plane — The total mass to pass across the plane of a grid cell (depicted by the thickness of the boxes) may vary because of differences in volumetric flow rate (size of arrows) resulting from aquifer heterogeneity and/or hydraulic stresses and differences in concentration (color of boxes with red = high, blue = low).*

5.0 Example Usage

5.1 Simple Example

A simple example application of the rtFlux software utility is presented here. The scenario involves a contaminant "spill" in a homogenous aquifer (represented by a single model layer) with a uniform gradient, as shown in Figure 10. The contaminant (e.g., vinyl chloride) undergoes aerobic degradation by aerobic direct metabolism. Thus, there are two chemical species (contaminant and oxygen) for RT3D to track. The simulation model is a single layer grid with 51 cells in the X direction and 31 cells in the Y direction. For this example four flux planes were specified in the X and Y directions as show in Figure 11. Figure 12 shows the plane definitions for these four flux planes. Figures 13 to 15 show standard RT3D results. The resulting concentrations of contaminant and oxygen after 730 days of the simulation are shown in Figures 13 and 14, respectively. Figure 15 shows time series plots for the concentrations of contaminant and oxygen at the observation location. Figures 16 through 19 show plots of the contaminant mass flow over time for planes 1 through 4, respectively, after post processing with the rtFlux utility. Figures 20 through 23 show plots of the oxygen mass flow over time for planes 1 through 4, respectively.

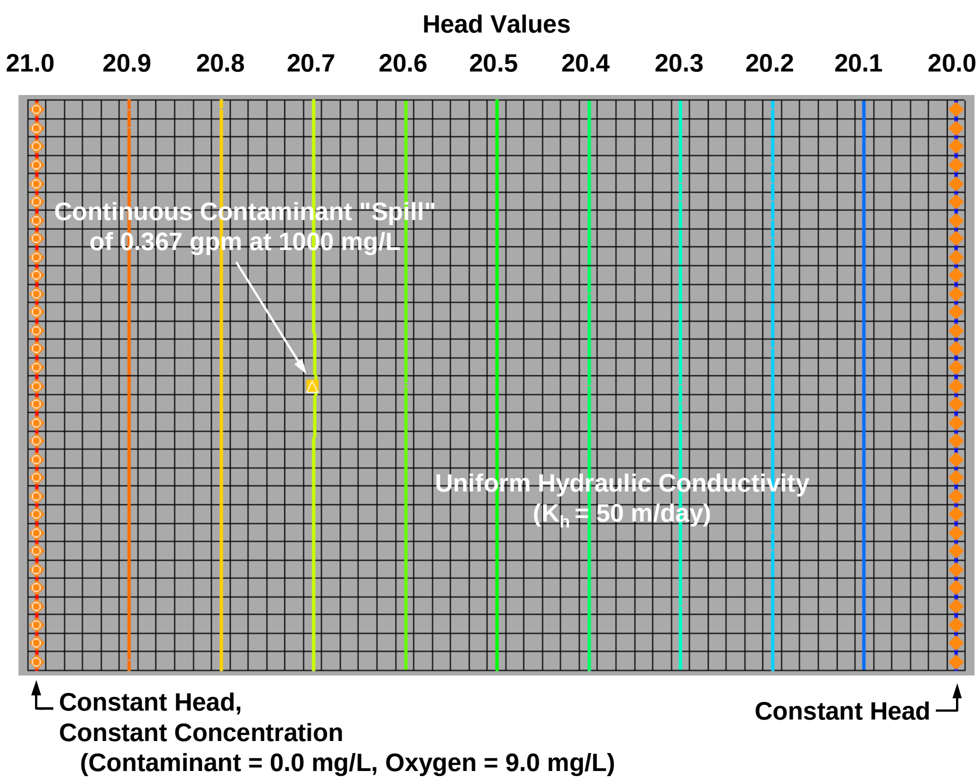

Figure 10. *The Scenario for the Simple Example Showing the Uniform Hydraulic Gradient, Boundary Conditions, and the "Spill" Location*

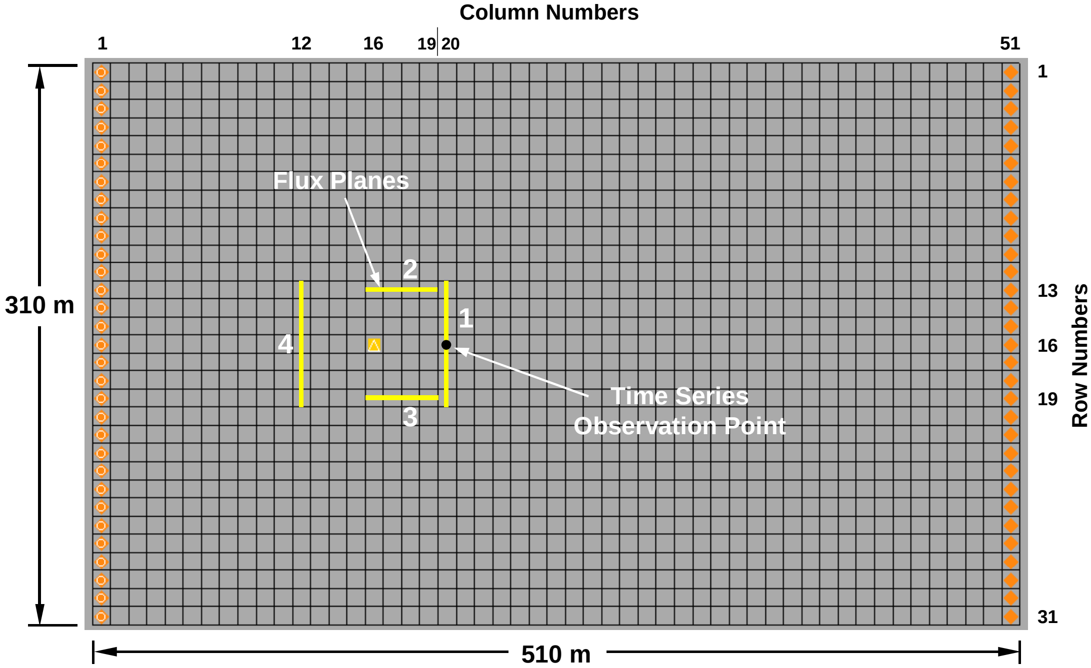

Figure 11. *Locations of the Four Flux Planes Used in the Simple Example and the Observation Point for Time Series Concentration Plots*

NCOL:	51
NROW:	31
NLAY:	1
Number of Planes:	4

BTN File:	
RT3D Superfile:	
LMKT Output File:	
IOB File:	

	Upper Left Corner Cell			Opposing Corner Cell				
Plane Identifier	COL	ROW	LAY	COL	ROW	LAY	Group ID	Plane Type
	20	19	1	20	13	1	1	YZ
	16	13	1	19	13	1	2	XZ
	16	20	1	19	20	1	3	XZ
	12	13	1	12	19	1	4	YZ

Figure 12. *Plane Definitions For The Planes Shown In Figure 11*

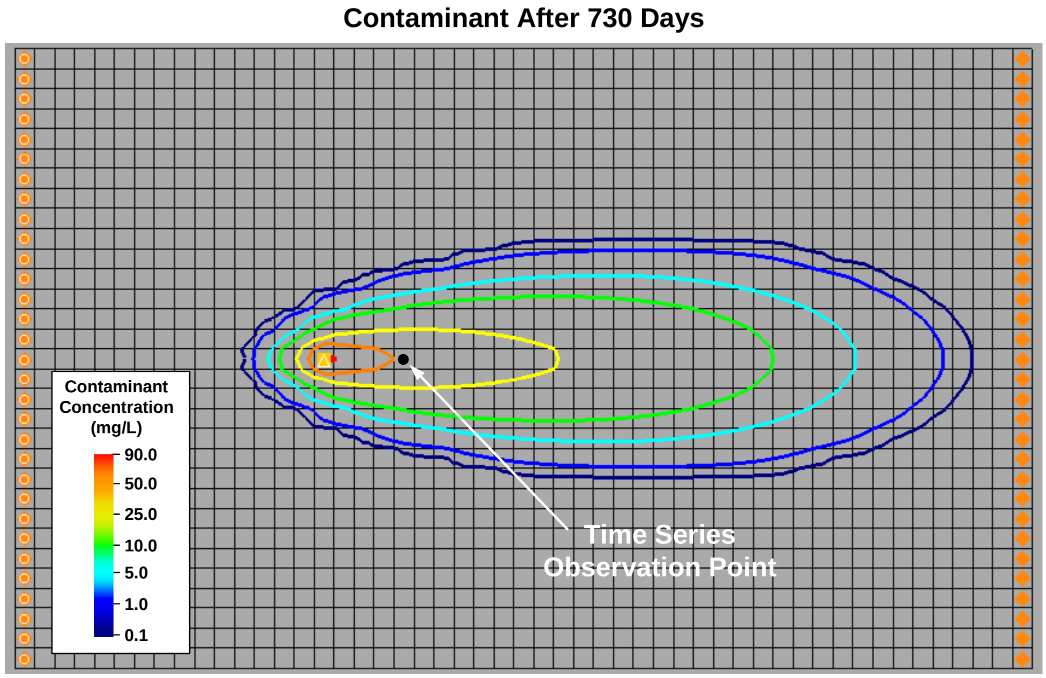

Figure 13. *Concentration Contours After 730 Days for the Contaminant Component*

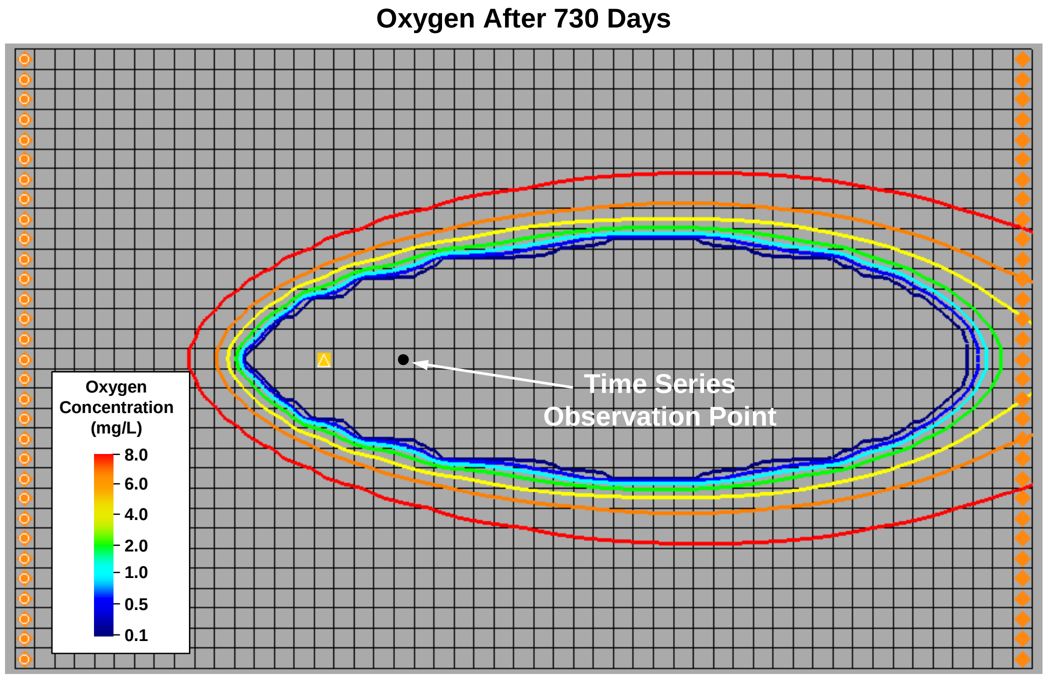

Figure 14. *Concentration Contours After 730 Days for the Oxygen Component*

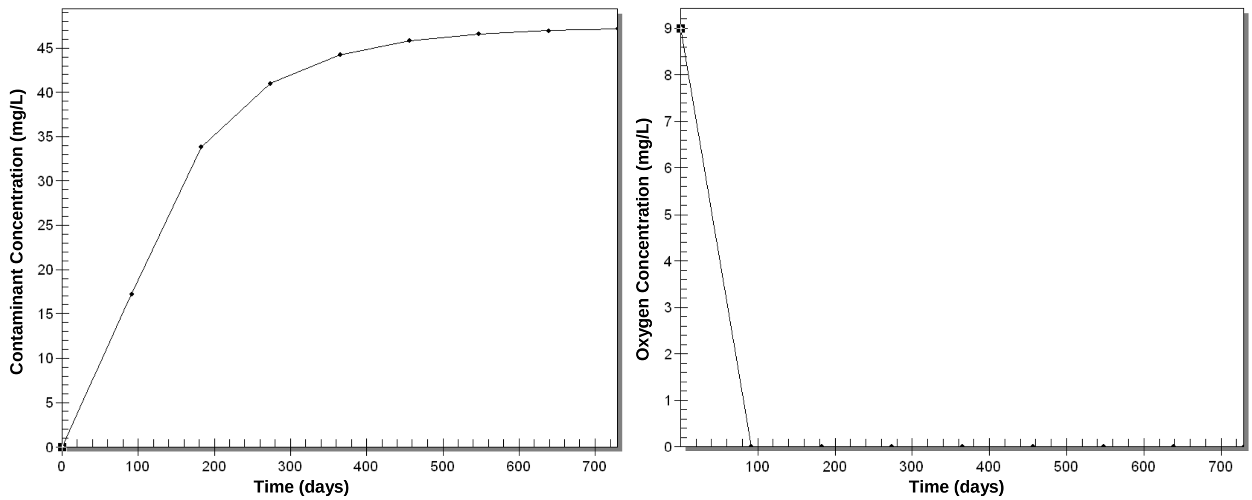

Figure 15. *Time Series Data Plots for Contaminant and Oxygen Concentrations at the Observation Point*

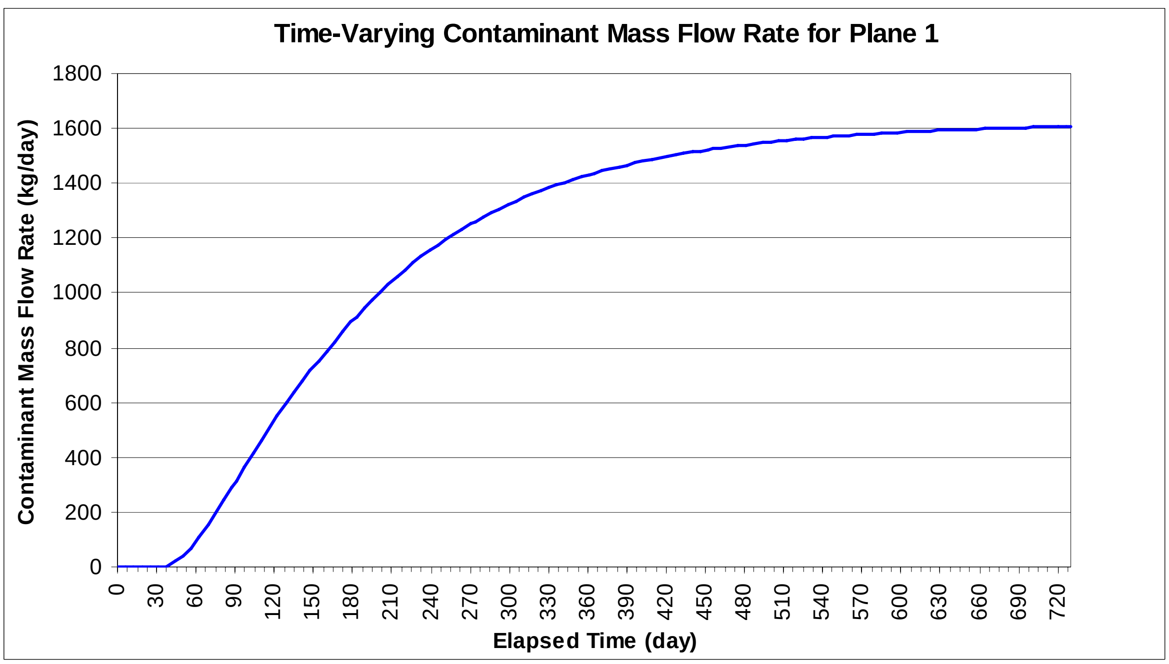

Figure 16. *Plot of the Mass Flow Rate of Contaminant Across Plane #1 as a Function of Time*

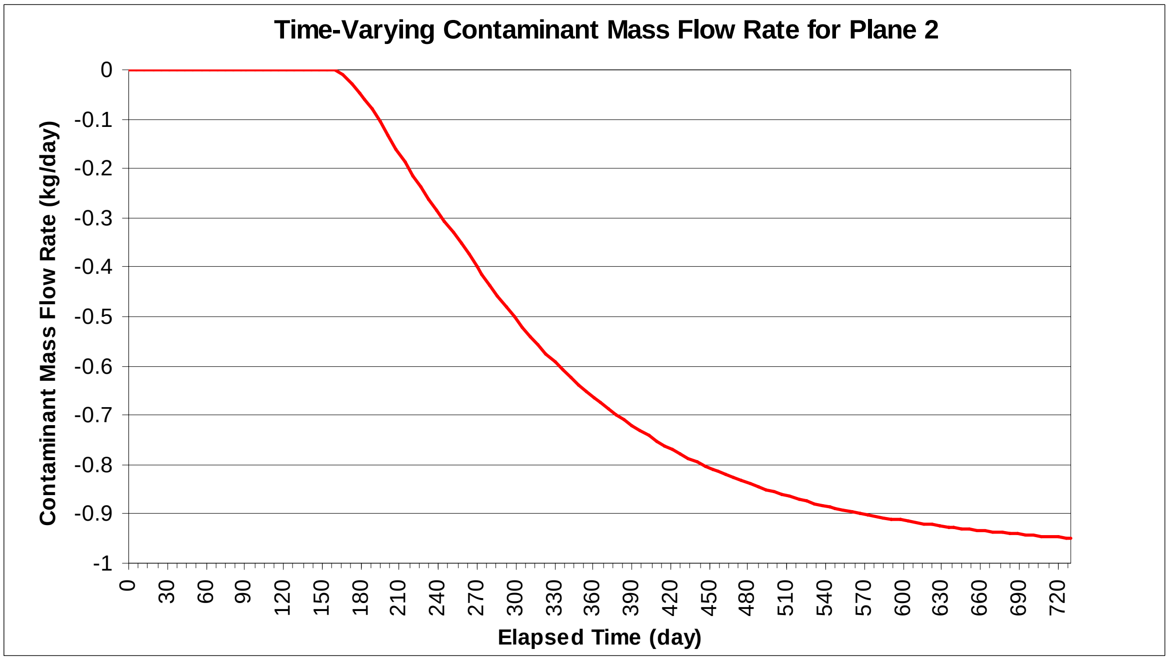

Figure 17. *Plot of the Mass Flow Rate of Contaminant Across Plane #2 as a Function of Time*

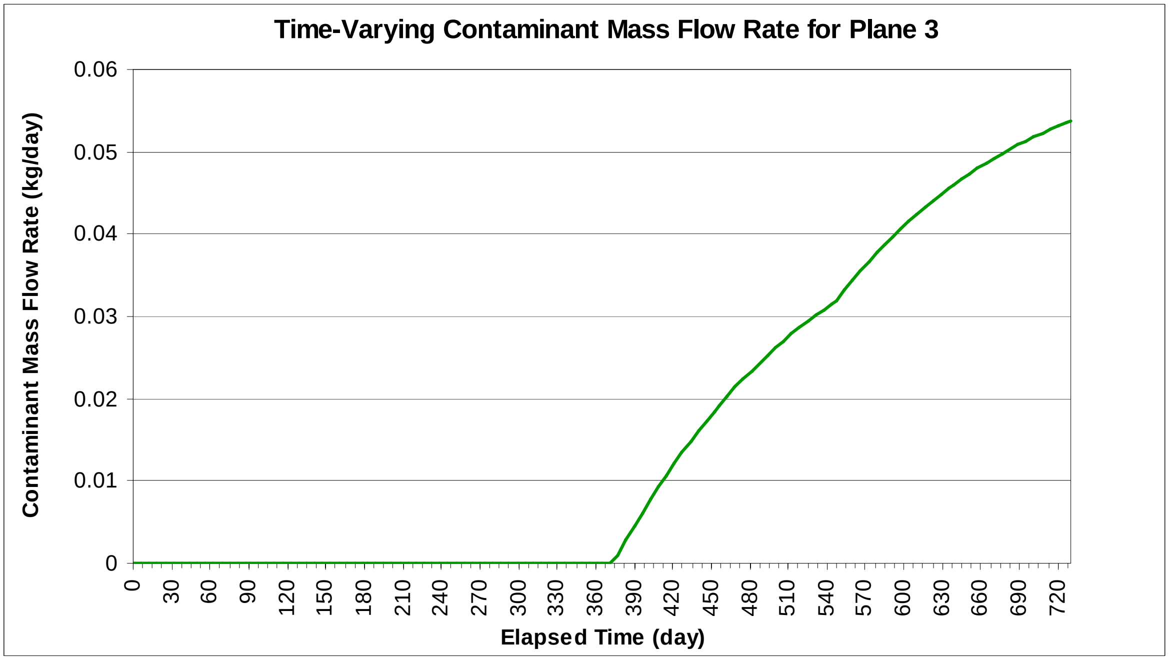

Figure 18. *Plot of the Mass Flow Rate of Contaminant Across Plane #3 as a Function of Time*

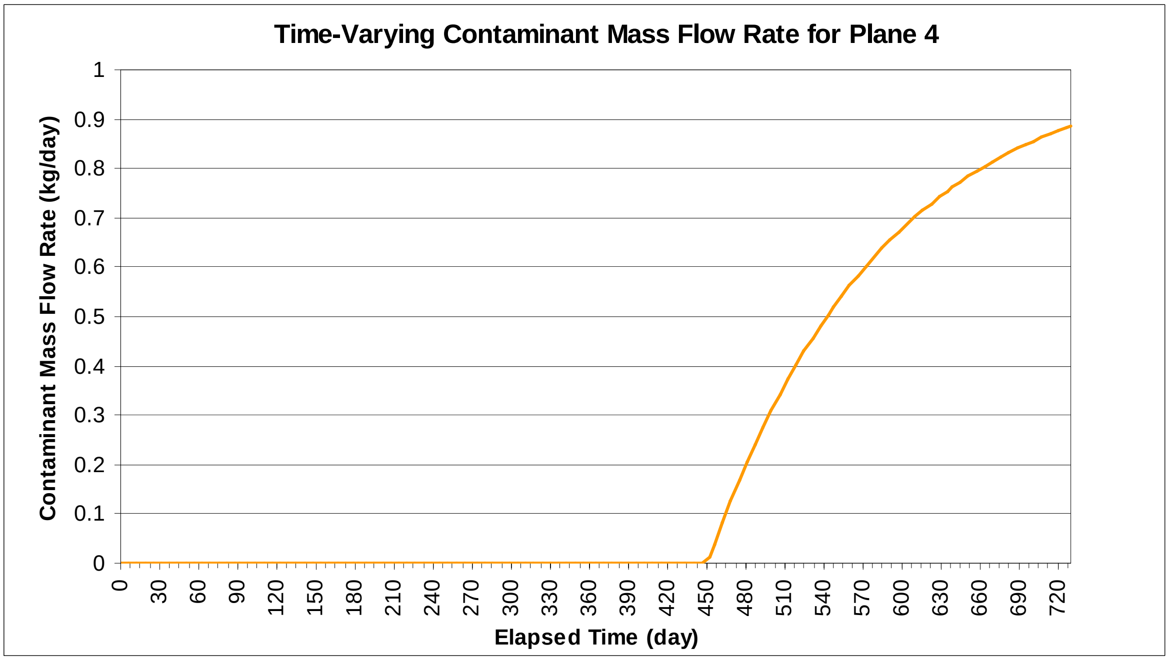

Figure 19. Plot of the Mass Flow Rate of Contaminant Across Plane #4 as a Function of Time

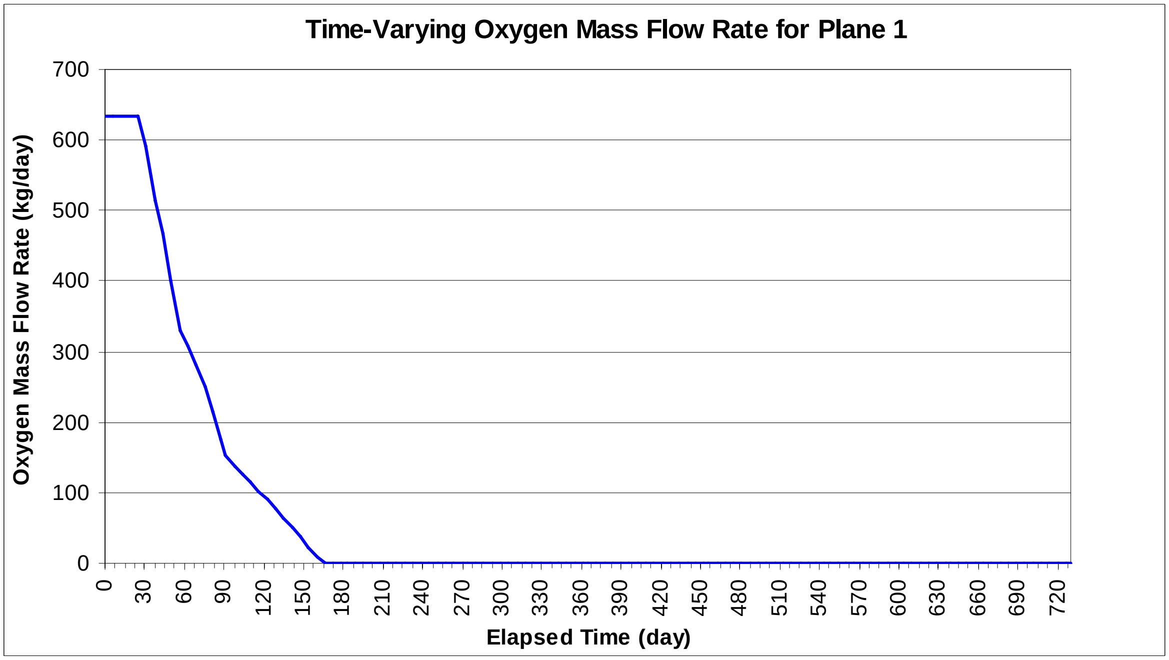

Figure 20. Plot of the Mass Flow Rate of Oxygen Across Plane #1 as a Function of Time

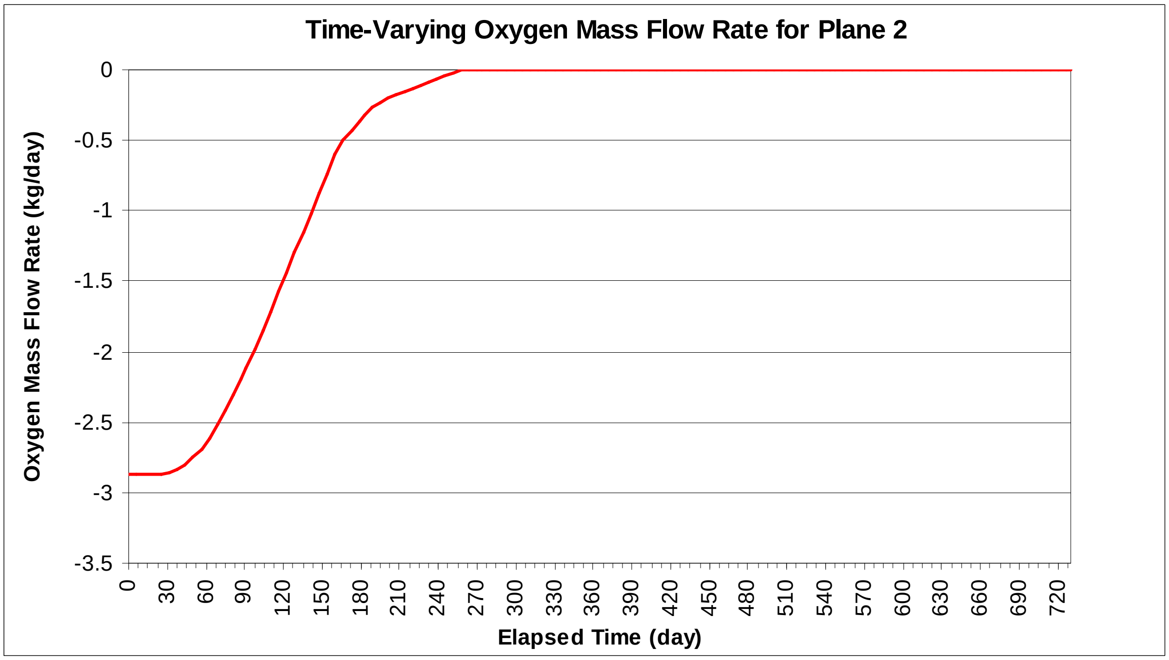

Figure 21. *Plot of the Mass Flow Rate of Oxygen Across Plane #2 as a Function of Time*

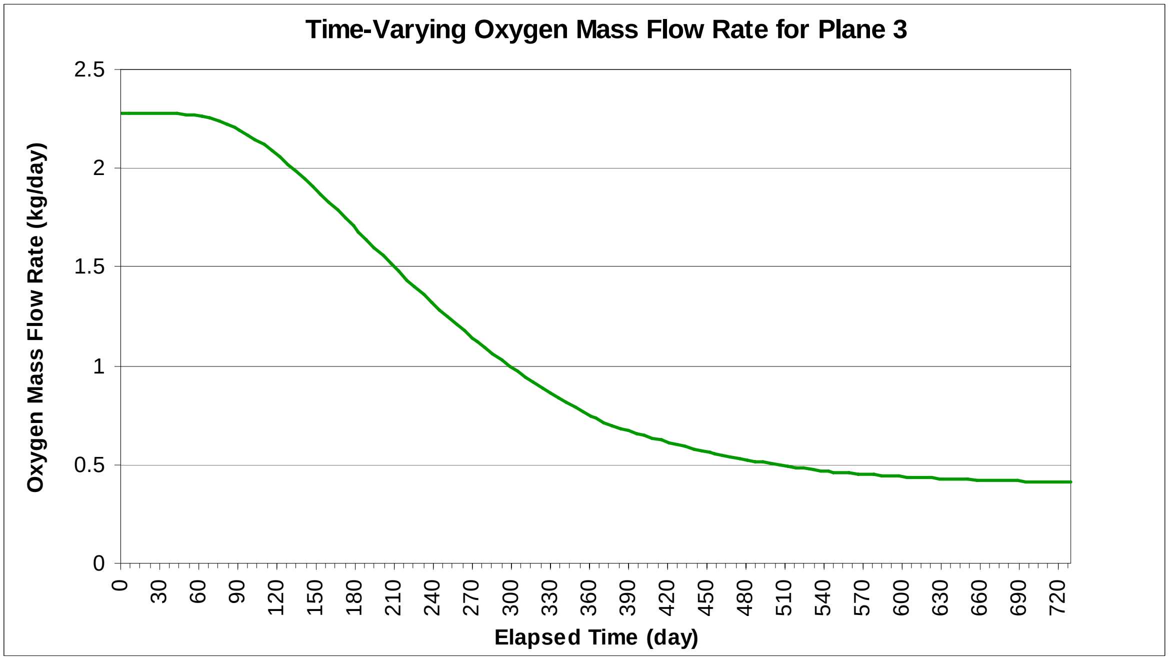

Figure 22. *Plot of the Mass Flow Rate of Oxygen Across Plane #3 as a Function of Time*

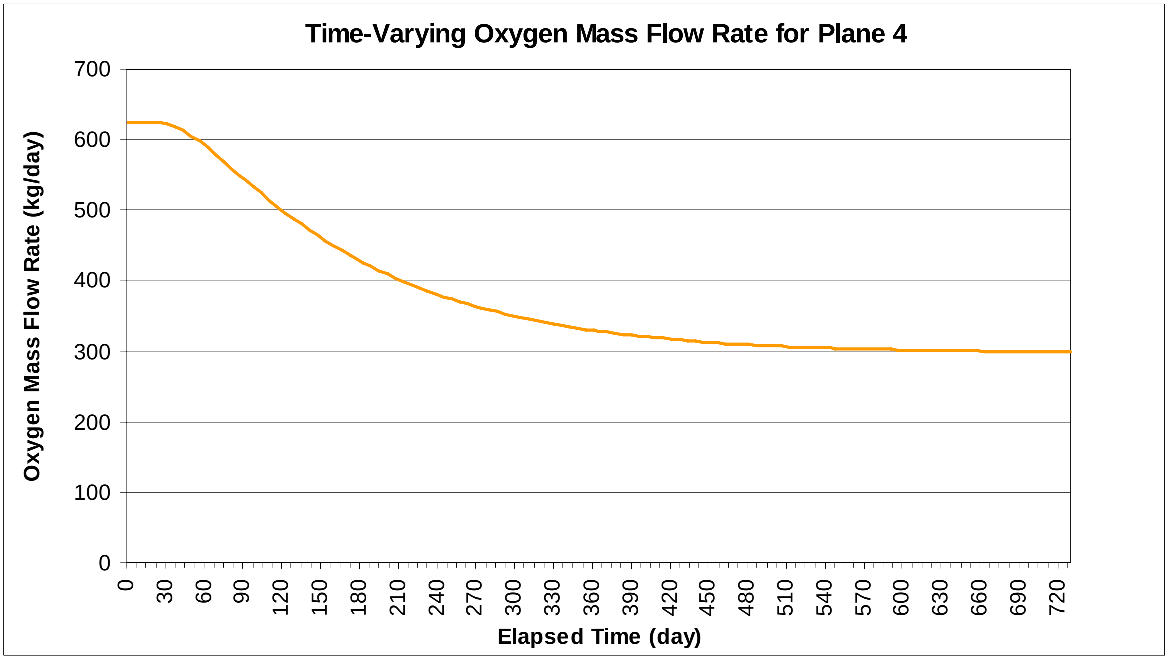

Figure 23. *Plot of the Mass Flow Rate of Oxygen Across Plane #4 as a Function of Time*

5.2 Multilayer Example

The simple example looked at the typical RT3D output, the configuration of flux planes, and the time series plots for mass flow. The multilayer example discussed in this section is more interesting with respect to the distribution of mass flow within the plane.

In this example, a rather large model is used to assess remediation scenarios for a single contaminant. The source area for the site has been removed, but a dissolved phase plume remains and is migrating downgradient towards receptors (Figure 24). Two simulations compare the results of natural attenuation processes (no active remediation) to the scenario of installing a pump-and-treat (P&T) system to intercept the bulk of the contaminant plume. The P&T system is operated for 25.5 years, then the residual plume is allowed to naturally attenuate. Several planes are defined (Figure 25), but plane #1 (located just downgradient of the P&T system) is of most interest for this comparison. The two scenarios were simulated using RT3D and the results were processed with the rtFlux utility. Figure 26 shows the mass flow rate and cumulative mass over time for plane #1. In the first scenario (no action) the mass flow through the plane is seen to increase as the core of the plume passes by the plane and then decrease because the contaminant source has been removed. In the second case, the P&T system effectively captures the dissolved contaminant plume, with the mass flow through the plane being about 15 times less than the "no action" scenario. When P&T is discontinued, the mass flow downgradient through the flux plane resumes. The cumulative mass plots are functions of the mass flow through the plane over time. For reference, contaminant contours for both scenarios are shown in Figure 27 at year 25.5.

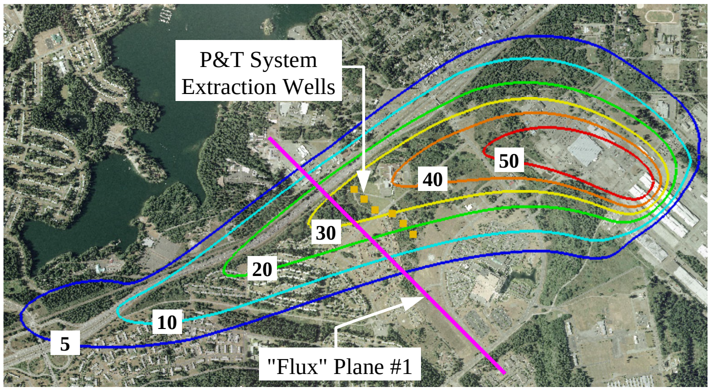

Figure 24. *Plan View of the Multilayer Example Showing Initial Conditions in Layer 33, the Location of Flux Plane #1, and the P&T Wells*

NCOL:	293
NROW:	216
NLAY:	46
Number of Planes:	5

BTN File:	
RT3D Superfile:	
LMKT Output File:	
IOB File:	

	Upper Left Corner Cell			Opposing Corner Cell				
Plane Identifier	COL	ROW	LAY	COL	ROW	LAY	Group ID	Plane Type
	123	137	27	190	137	46	1	XZ
	109	166	28	109	193	46	2	YZ
	224	68	1	224	125	15	3	YZ
	196	68	1	196	125	15	4	YZ
	152	68	1	152	125	25	5	YZ

Figure 25. *Definition of the Planes for the Multilayer Example*

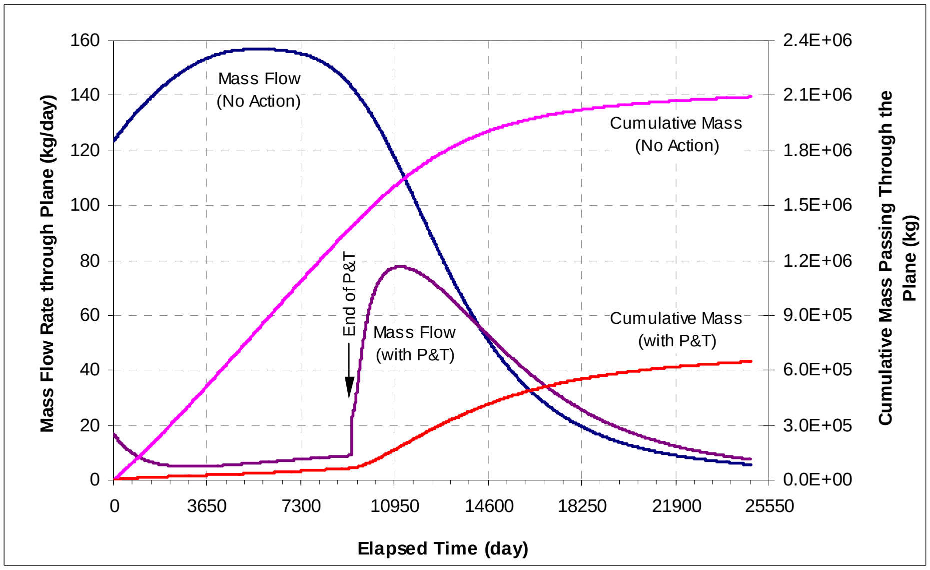

Figure 26. *Mass Flow Rate and Cumulative Mass to Pass Through a Plane for the Two Scenarios of the Multilayer Example — In one case no action is taken (natural attenuation only) and in the other P&T is applied. In both cases, the non-aqueous phase liquid source was removed.*

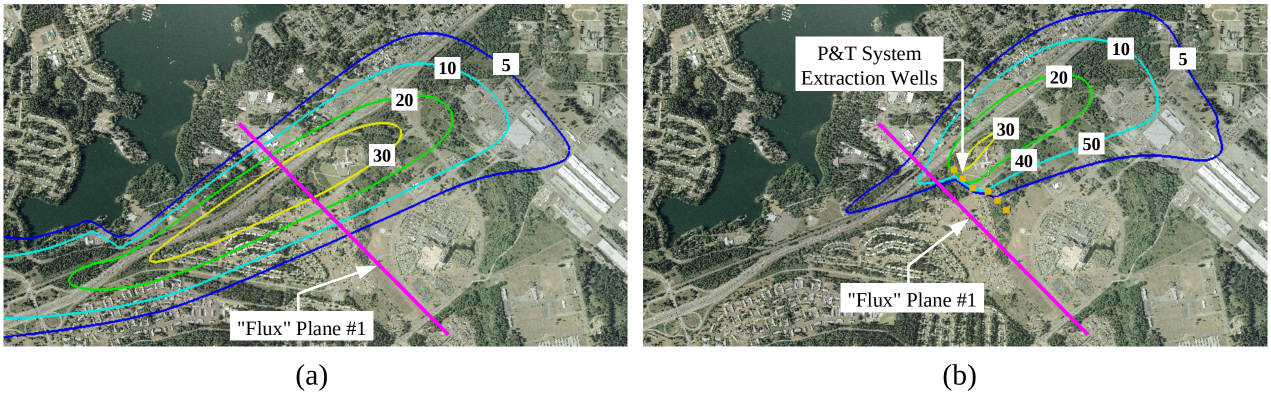

Figure 27. *Contaminant Contours (µg/L) After 25.5 Years for the Scenarios of (A) Natural Attenuation Only and (B) Pump-And-Treat; the Pump-And-Treat System Was Discontinued After this Time*

Data for bubble plots are available at regular time intervals. As an example, Figures 28 to 30 show the bubble plots of the volumetric flow rate, contaminant concentration, and mass flow rate, respectively, at an elapsed time of 10000 days (~27 years) in plane #1 for the natural attenuation only scenario. The displayed extent of plane #1 has been cropped to just beyond the extent of the plume for presentation purposes. Above layer 31 there is a clay confining layer, which is apparent from the grid cells with much smaller or no bubbles for volumetric flow (Figure 28). A similar low conductivity zone exists in the bottom layers. The volumetric flow is relatively uniform within each of several zones of differing hydraulic conductivity. The contaminant concentration (Figure 29) is distributed laterally around a high concentration core near the center of the flux plane. The mass flow (Figure 30) is the product of the volumetric flow rate and the concentration, thus exhibits a distribution with the highest mass flows at the points of high concentration and high volumetric flow rate.

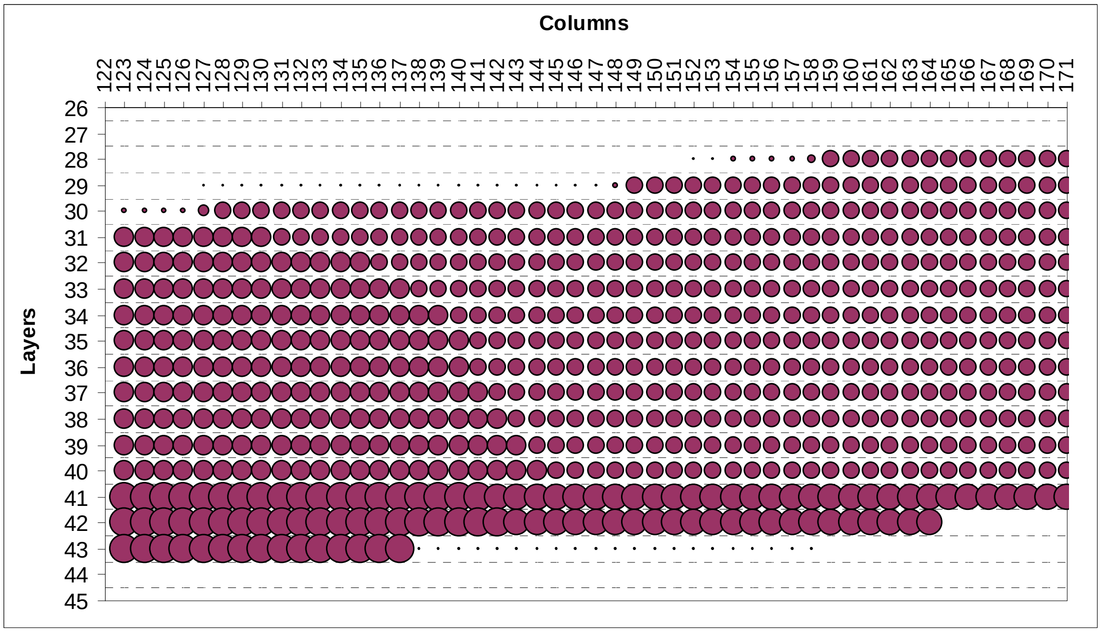

Figure 28. *Relative Volumetric Flow Rate (e.g., ft^3/day) at Flux Plane #1 on Simulation Day 10000 of the Multilayer Example "No Action" Scenario*

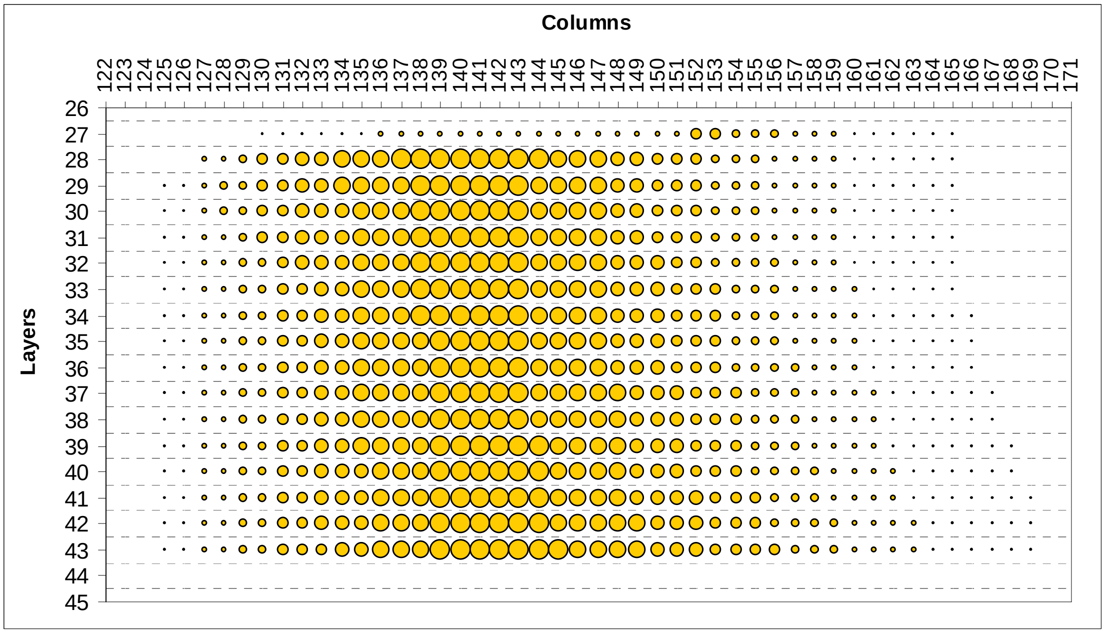

Figure 29. *Relative Contaminant Concentration (mg/L) at Flux Plane #1 on Simulation Day 10000 of the Multilayer Example "No Action" Scenario*

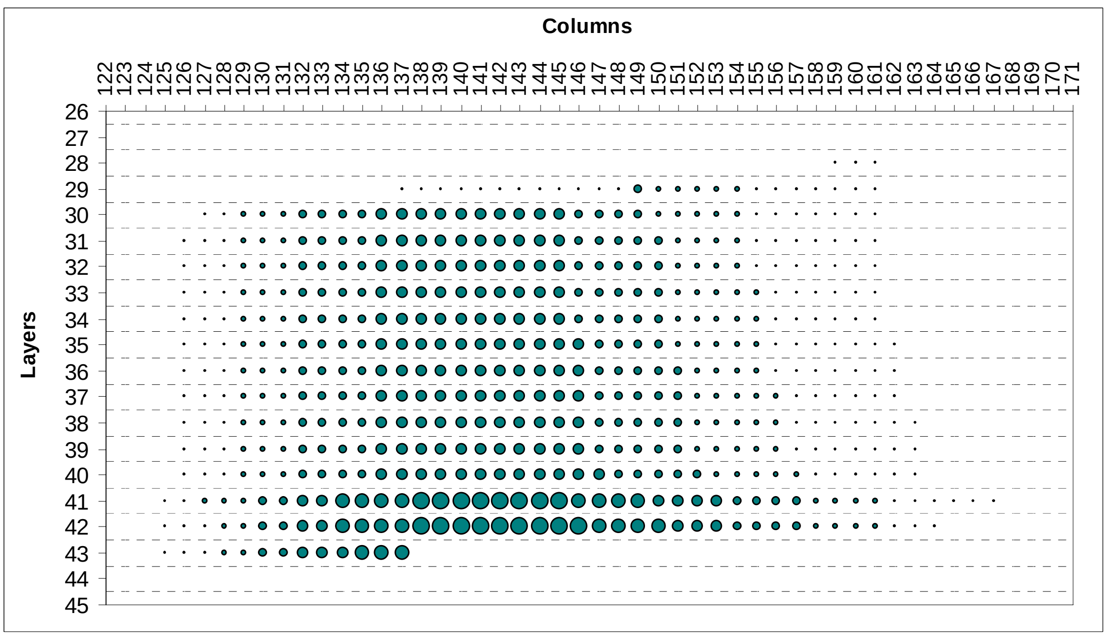

Figure 30. *Relative Mass Flow Rate (kg/day) at Flux Plane #1 on Simulation Day 10000 of the Multilayer Example "No Action" Scenario*

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