User's Manual

for the Fate and Transport Software Developed by Eco

by

Zurab Khviengia

Research Department, Eco & Associates, Inc.

1855 W. Katella Ave, Suite 350, Orange, CA 92867

zkhviengia@ecoinc.info

Phone: 1(714)289-0995 Fax: 1(714)289-0965

Abstract

This is a brief description of the functional part of the software developed by Eco. This Microsoft Excel based graphical software is designed for groundwater contamination analysis for the sites with extended, irregular sources. The input consisting of the sampling data from multiple monitoring wells located around the perimeter of the contaminated site generates the output that provides concentration values on the grid that can be set up arbitrarily and is one of the parameters that user has to input. The generated output then is plotted on a three-dimensional graph. This pictorial representation of the plume when generated for consecutive moments of time can then be combined into the dynamic animated picture of the plume evolution Most of the software applications available today that perform similar analysis make certain assumptions about the plume or the source that generates it, restricting them to a certain behavior or a configuration. Given software is probably the most general in this regard. The only restriction it has is the assumption inherent to all analytical models, - that the groundwater velocity is constant, the sorption is linear and the biodegradation is of the first order. It also assumes that the dispersion coefficients are constant and that there are no sinks or external sources within the area of analysis. These are natural assumptions that do not hinder analysis and can hardly be avoided in any analytical model. This is a good tool for preliminary analysis; is very simple to use and intuitive to understand.

Introduction

This software was developed as the aid in one of Eco's projects to analyze the plume of contaminated groundwater. Many parameters used in this software – their range and particular values – are taken from the data obtained at that site. The software has not been tested for other sets of parameters and different choices of their values. Eco offers this software to everybody interested in optimizing data analysis for their sites. The software is novel and has no analogs on the market today. It can easily be adjusted to similar projects, or be modified to incorporate new site configurations and different in character sampling data.

1 Main Functional Features

The main part of this software calculates concentrations on the grid provided for it by the user. The coordinates for the grid will necessarily depend on the particular configuration of the site, its size and the area in which the plume evolution is considered. For each point on the grid, the concentration is calculated according to the analytical formula derived by the author. The calculation is carried in the background and the results are displayed in the excel table.

The next functional part of the software prepares a table in the format required by the three-dimensional surface plot in excel. It builds this table based on the original coordinates of the grid and calculated for them concentrations. While the original table and the grid can be three-dimensional , contain (x, y, z) coordinates, this table accepts only two coordinates and therefore one variable, most frequently z, has to be specified as constant. Then the table displays the values of concentration corresponding to the planar (x, y) coordinates. This data is automatically displayed on the 3D surface graph, which depicts the plume in three dimensions across the area specified by the grid.

The above considered two functions are the two main functions that this software provides for the reader.

2 Additional Functional Features

In real life, it often becomes important to have a good pictorial representation of the data collected form the monitoring wells at the site. As an additional feature, this software plots the sampling data as a three-dimensional bar chart on the same grid on which the monitoring wells can be displayed. This enables the user to review the sampling data from all monitoring wells simultaneously and also view their evolution in time.

One more tool that the software provides for the user is the ability to view the source well concentrations as the synchronized in 3D strip charts, so called 3D line charts. This facilitates the understanding of the source behavior, the distribution of the concentration across it, as well as its dynamics.

These two auxiliary tools are mostly pictorial and do not involve any extended analytical calculations based on the model.

3 The Parameter Input Worksheet

This worksheet is where all parameters have to be input. Below are given brief descriptions of the parameters and the corresponding tables they are entered into.

3.1 Table 1: Groundwater Characteristics

This is the table that contains the groundwater velocity and the coefficients of dispersion in the x-, y-, z-directions. The table is displayed below:

Fig.1. Groundwater Characteristics Table

V	Dx	Dy	Dz
7	200	150	0.2

The groundwater velocity V is assumed to be constant. Groundwater is assumed to be flowing linearly with a steady flow. This is a common restriction for all analytical models. Irregularities in V or the direction of the flow are hard to be accounted for analytically and thus are rarely considered within the framework of analytical modeling.

Dispersion in the x-, y-, z-directions is assumed to be dynamic and , in general, different for each odrection. Therefore, Dx, Dy and Dz coefficients can, in general, be unequal in the table above. By making the dispersion to be close to zero one can account effectively for directional restrictions and make the three-dimensional flow effectively to be two- or one-dimensional.

3.2 Table 2: Bio-Chemical Characteristics

For our model, which is developed only for a single chemical compound, this table contains only one row: biodegradation constant of a given chemical. (See below)

Fig.2. Chemical Characteristics Table

Lambda	1.00E-07

Biodegradation is this model global in character: this constant does not depend on the coordinates. A change in this constant changes the concertation globally, at each point of the considered area. In many cases this constant does not play a crucial role in conducting the analysis if the chemical under consideration is relatively stable and hence has a very small biodegradation constant.

3.3 Table 3: Step

This constant is not related to groundwater. It is a model-based constant that is sensitive to the overall scale of the problem. This constant defines integration increment for numerical calculations since the formula utilized in the model contains the integration over time. The smaller this constant,

the closer the numerical value of the integral is to its analytically calculated value. For the considered problem this value is chosen to be 0.1, which translates approximately to 1000 iterations for the integration. This value of the step achieves desirable accuracy in the problem.

Fig.3. Variables Table

step	0.1

Further decrease of this parameter for the given problem has almost no effect on concentration values calculated for the grid.

3.4 Table 4: Source Wells

This is a simple table displaying the number of source wells for which the sampling data is provided on the data sheet (worksheet 2).

Fig.4. Source Wells Table

Number	9

In the design of the model, the source wells are taken to be located around the perimeter of the contaminated site. Their number is not restricted. These are the wells for which the sampling data are collected and used by the software. The more wells we have here, the more accurate the analysis is going to be.

3.5 Table 5: Source Well Coordinates and Boundaries

This table specifies spatial coordinates for each source well by specifying the patch dimensions and coordinates for each of them. (See below)

Fig.5. Source Well Coordinates and Boundaries Table

	PWB-6	PWB-2	WB2-2	PWB-4	AR-1	WB2-1	AMW-4R	PWB-3	PWB-1
X0	225	400	175	325	0	500	275	550	225
Y1	-500	-300	-100	-50	-25	25	250	375	400
Y2	-300	-100	-50	-25	25	250	375	400	425
Z1	0	0	0	0	0	0	0	0	0
Z2	-5	-5	-5	-5	-5	-5	-5	-5	-5

The parameter Xo specified the x-coordinate of the wells (The origin of the coordinate system is more or less arbitrary and can be taken to coincide with one of the wells; in the above example with AR-1 well). Y1 and Y2 are the transverse coordinates of the patch associated with the wells. The choice of the patch depends on the researcher. The concertation within that patch is assumed to be constant in the model. The smaller the patch, the less the influence of that particular well on the

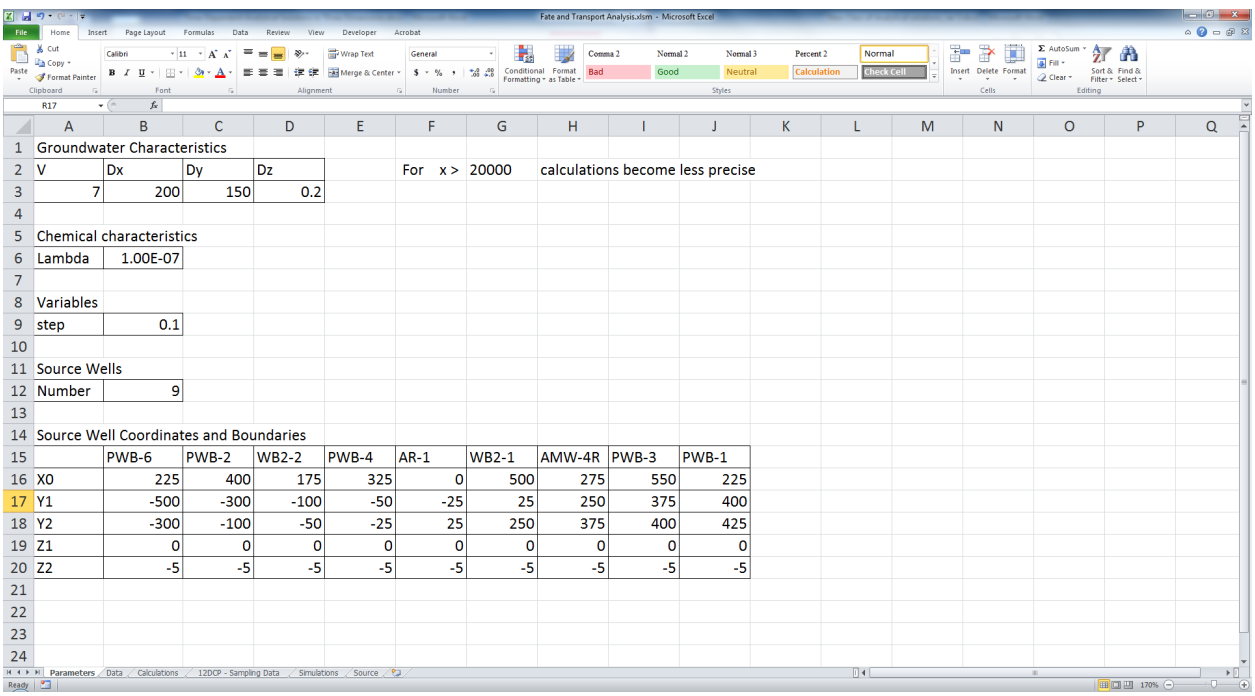
overall distribution of concentration. Z1 and Z2 provide corresponding Z-coordinates of those patches.

This table is very site specific. It depends on the geometric size of the site as well as on the particular distribution of the source well. The final result may not be sensitive to the slight variations in the values of the listed in this table parameters.

3.6 Commentary

Due to the complex analytical nature of the model applied in this software, the calculations conducted in the background may overrun the memory provided by Excel, reaching too large in magnitude numbers, and potentially running the risk of crushing the application. To prevent this from happening, a recommended range for the linear variable x (coordinate along the flow of groundwater) has to be specified. This value is affected by the ratio of the coefficient of dispersion in the x direction Dx over the magnitude of the velocity V. For a given problem, it is approximately 20 000 which is far beyond the considered area of interest where the plume evolution is calculated.

Fig.6. "Parameters" worksheet



	A	B	C	D	E	F	G	H	I	J
1	Groundwater Characteristics									
2	V	Dx	Dy	Dz		For x >	20000	calculations become less precise		
3	7	200	150	0.2						
4										
5	Chemical characteristics									
6	Lambda	1.00E-07								
7										
8	Variables									
9	step	0.1								
10										
11	Source Wells									
12	Number	9								
13										
14	Source Well Coordinates and Boundaries									
15		PWB-6	PWB-2	WB2-2	PWB-4	AR-1	WB2-1	AMW-4R	PWB-3	PWB-1
16	X0	225	400	175	325	0	500	275	550	225
17	Y1	-500	-300	-100	-50	-25	25	250	375	400
18	Y2	-300	-100	-50	-25	25	250	375	400	425
19	Z1	0	0	0	0	0	0	0	0	0
20	Z2	-5	-5	-5	-5	-5	-5	-5	-5	-5

4 The Data Worksheet

This worksheet provides the sampling data in the concentration vs time form. The time is calculated in months, but, in general, can be measured in any temporal units. The data are arranged vertically by the columns corresponding to each source well. The fragment of this table for the first few source wells is shown below.

Fig.7. “Data” Worksheet

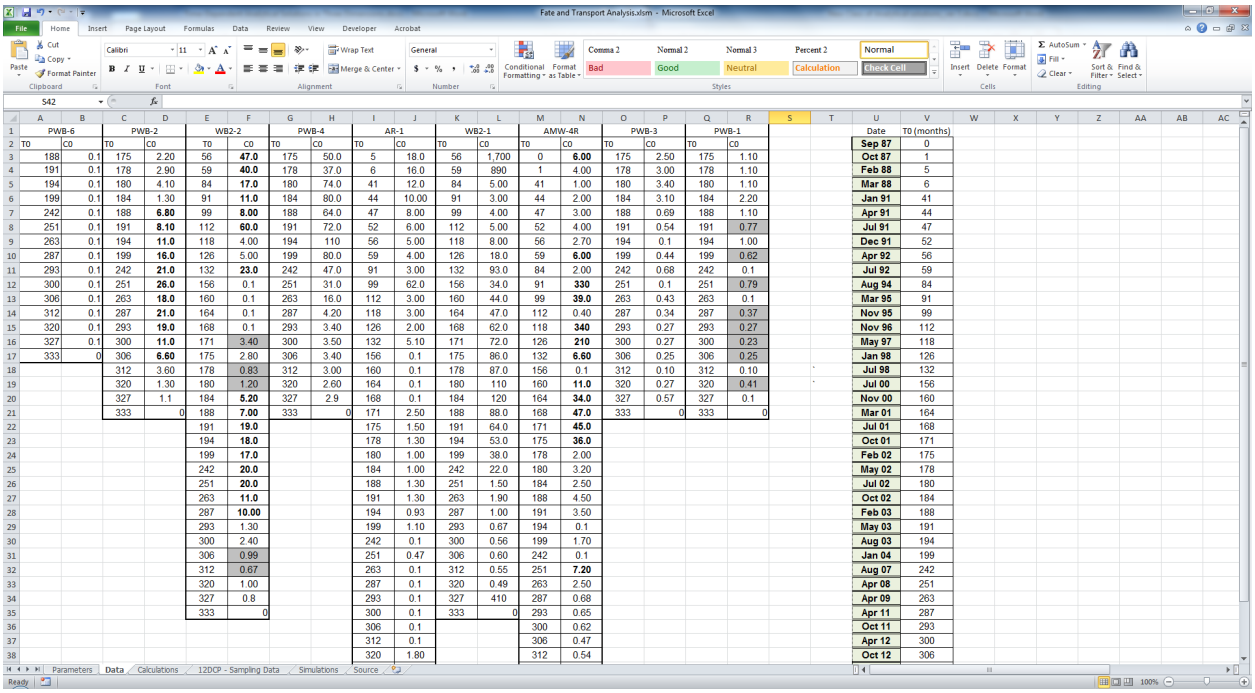
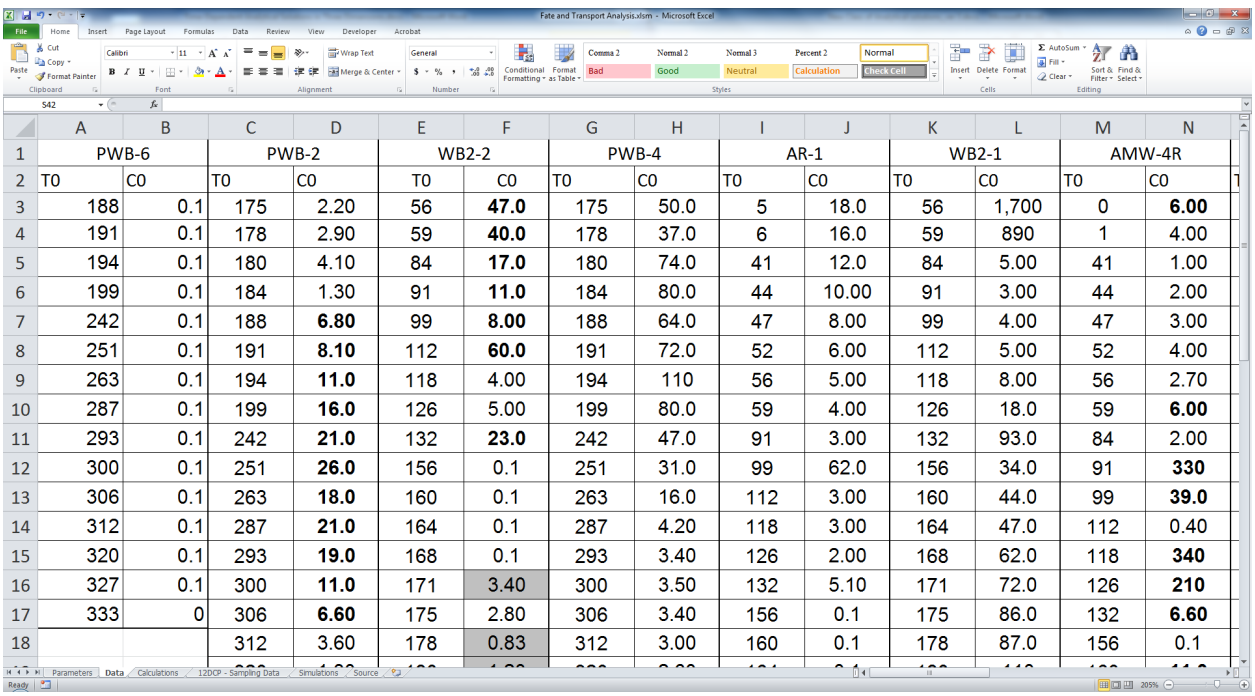


Fig.8. Fragment of the Data Table



PWB-6		PWB-2		WB2-2		PWB-4		AR-1		WB2-1		AMW-4R	
T0	C0	T0	C0	T0	C0	T0	C0	T0	C0	T0	C0	T0	C0
188	0.1	175	2.20	56	**47.0**	175	50.0	5	18.0	56	1,700	0	**6.00**
191	0.1	178	2.90	59	**40.0**	178	37.0	6	16.0	59	890	1	4.00
194	0.1	180	4.10	84	**17.0**	180	74.0	41	12.0	84	5.00	41	1.00
199	0.1	184	1.30	91	**11.0**	184	80.0	44	10.00	91	3.00	44	2.00
242	0.1	188	**6.80**	99	**8.00**	188	64.0	47	8.00	99	4.00	47	3.00
251	0.1	191	**8.10**	112	**60.0**	191	72.0	52	6.00	112	5.00	52	4.00
263	0.1	194	**11.0**	118	4.00	194	110	56	5.00	118	8.00	56	2.70
287	0.1	199	**16.0**	126	5.00	199	80.0	59	4.00	126	18.0	59	**6.00**
293	0.1	242	**21.0**	132	**23.0**	242	47.0	91	3.00	132	93.0	84	2.00
300	0.1	251	**26.0**	156	0.1	251	31.0	99	62.0	156	34.0	91	**330**
306	0.1	263	**18.0**	160	0.1	263	16.0	112	3.00	160	44.0	99	**39.0**
312	0.1	287	**21.0**	164	0.1	287	4.20	118	3.00	164	47.0	112	0.40
320	0.1	293	**19.0**	168	0.1	293	3.40	126	2.00	168	62.0	118	**340**
327	0.1	300	**11.0**	171	3.40	300	3.50	132	5.10	171	72.0	126	**210**
333	0	306	**6.60**	175	2.80	306	3.40	156	0.1	175	86.0	132	**6.60**
		312	3.60	178	0.83	312	3.00	160	0.1	178	87.0	156	0.1

5 The Calculation Worksheet

This is the main functional worksheet of this software. The columns (x, y ,z, t) give the grid coordinates and the time for which the concentration is calculated in the last column. Time here should be measured in the same units as in the table above. The coordinates should also be consistent with the units in which the source well patches are given in the table 5. The size of the grid is the choice of the user. For a given problem, this table contains over one thousand rows for each specific time value. But, in general, fewer number of grids can be specified in a problem.

After populating the table, one clicks on the "Calculate" button and the values of C(x, y, z, t) are filled in as a result of background calculations. The code is written as a VBA macro to which this button is linked to. The calculation may take a few minutes depending on the data volume.

Fig.9. Concentration Calculation Table

				Calculate Clear
x	y	z	t	C(x, y, z, t)
500	-500	0	362	0.028403
600	-500	0	362	0.077629
700	-500	0	362	0.179131
800	-500	0	362	0.327329
900	-500	0	362	0.482842
1000	-500	0	362	0.604975

After the calculations are finished, one clicks on the "Graph" button and the reformatted data are first re-arranged into the 3D-graph table and then automatically plotted on the graph too.

Fig.10. Graph Data Table

Graph Clear		-500	-450	-400	-350	-300	-250
	500	0.028403	0.046949	0.073301	0.108102	0.149985	0.195972
	600	0.077629	0.13793	0.227535	0.345363	0.480851	0.623306
	700	0.179131	0.317522	0.518071	0.772978	1.054999	1.342419
	800	0.327329	0.562604	0.890393	1.291422	1.71664	2.116504
	900	0.482842	0.799217	1.223684	1.726526	2.242243	2.691132

Corresponding "Clear" buttons clear the areas and prepare them for new calculations.

Fig.11. “Calculations” Worksheet before calculations are performed.

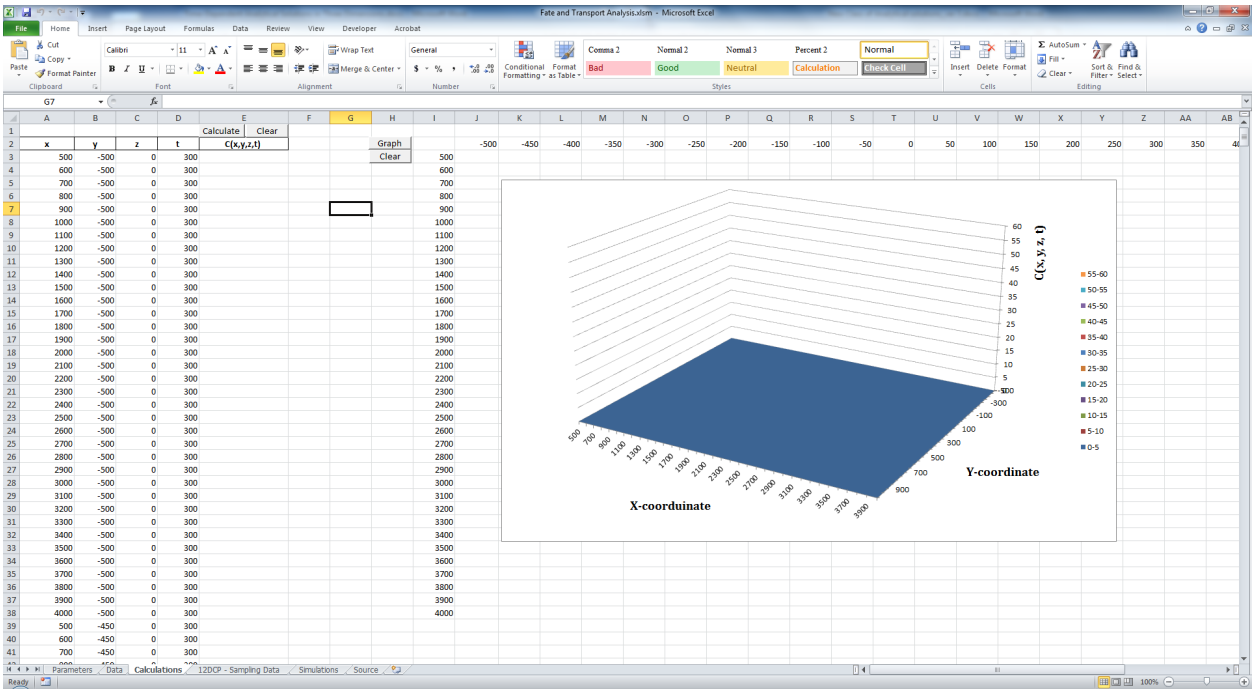
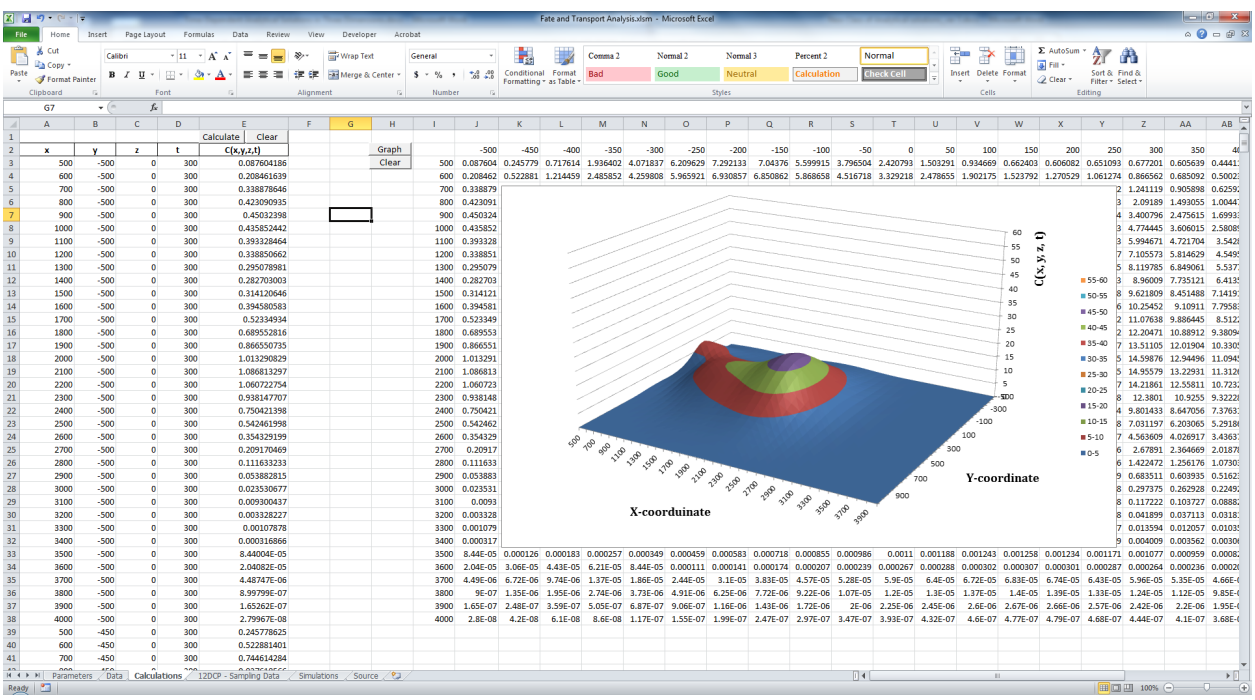


Fig.12. “Calculations” Worksheet after the calculations and graphing.



6 Auxiliary Graphs

6.1 Sampling Data Graph

This graph depicts the sampling data for the wells located below the source wells, where the main plume is analyzed in the problem, - this is the area covered by the software. (See below). By selecting a corresponding sampling date in the drop down menu of the Date field (the uppermost first cell on the worksheet), one automatically plots the data for that particular date.

Fig.13. "12DCP – Sampling Data" Worksheet

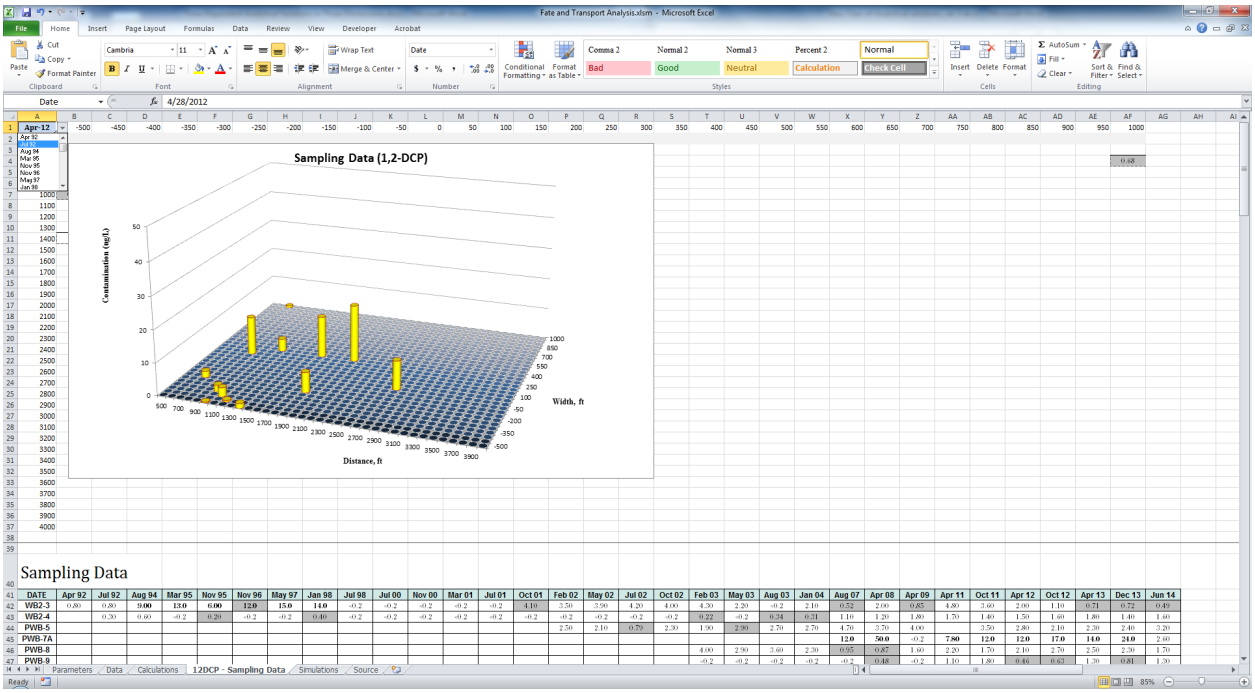
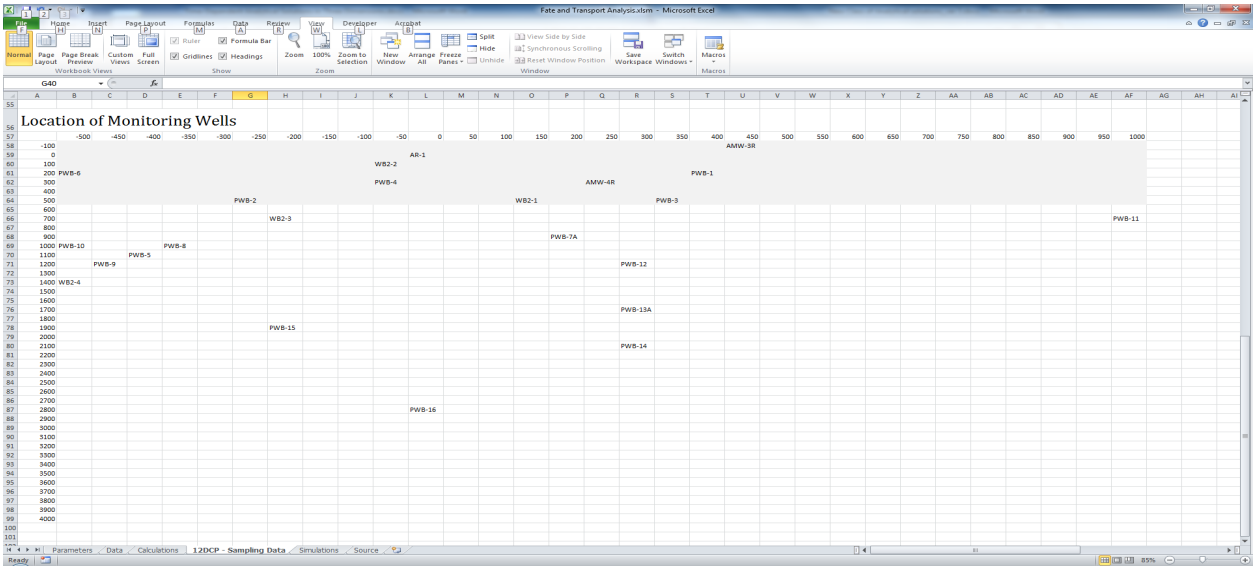


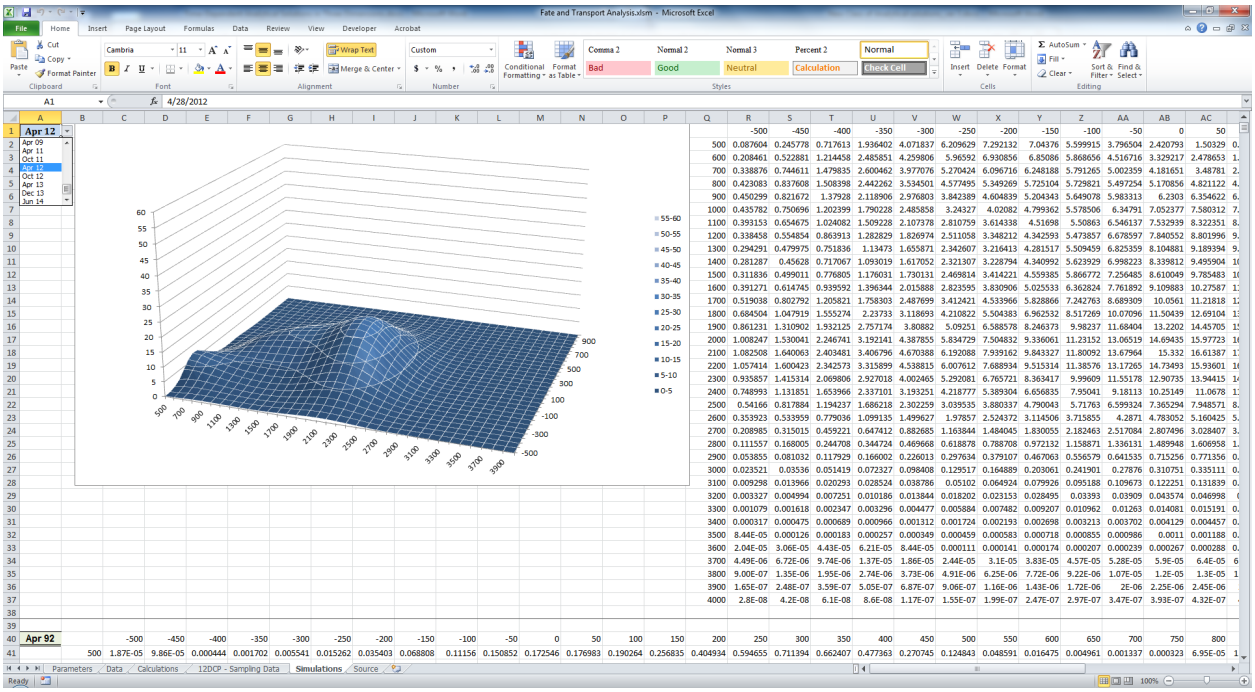
Fig.14. Location of Monitoring Wells Table on the Same Worksheet



6.2 The Simulations Worksheet

This worksheet collects the grid concertation tables for all sampling events obtained from the "Calculations" worksheet. This enables the user to select a corresponding date on the drop down menu and immediately view the concentration vs plume area 3D graph (see below). These graphs are identical to the graphs that could be obtained on the Calculation worksheet. However, here all these graphs can be depicted at once, without waiting for the calculations to finish, which that sometimes can take several minutes.

Fig.15. "Simulations" Worksheet



6.3 The Source Well Sampling Data Graph

The data provided on the Data worksheet (Worksheet 2) is deployed on this worksheet ("Source" worksheet) as a three-dimensional strip chart. (See below).

This chart is approximate, it ignores the effects of dispersion and biodegradation within the source area. If all wells were aligned across the groundwater flow, than this chart would be an exact representation of spatial distribution of the concentration.

Fig.16. “Source” Worksheet

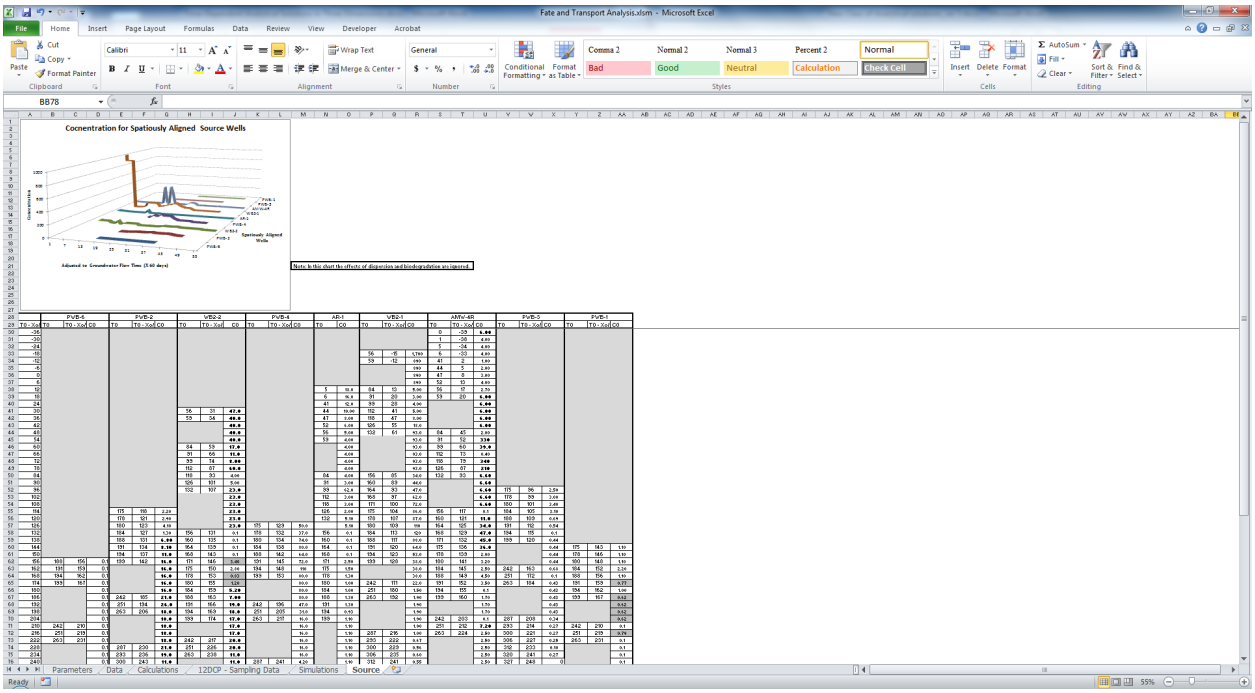
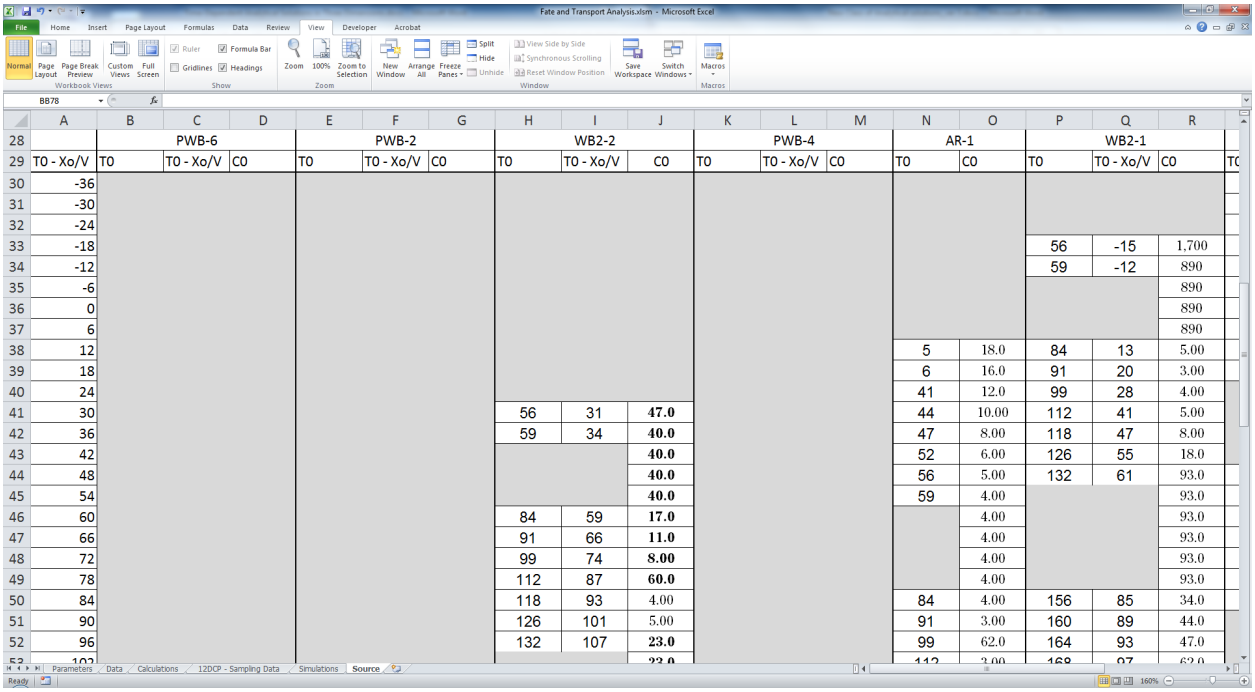
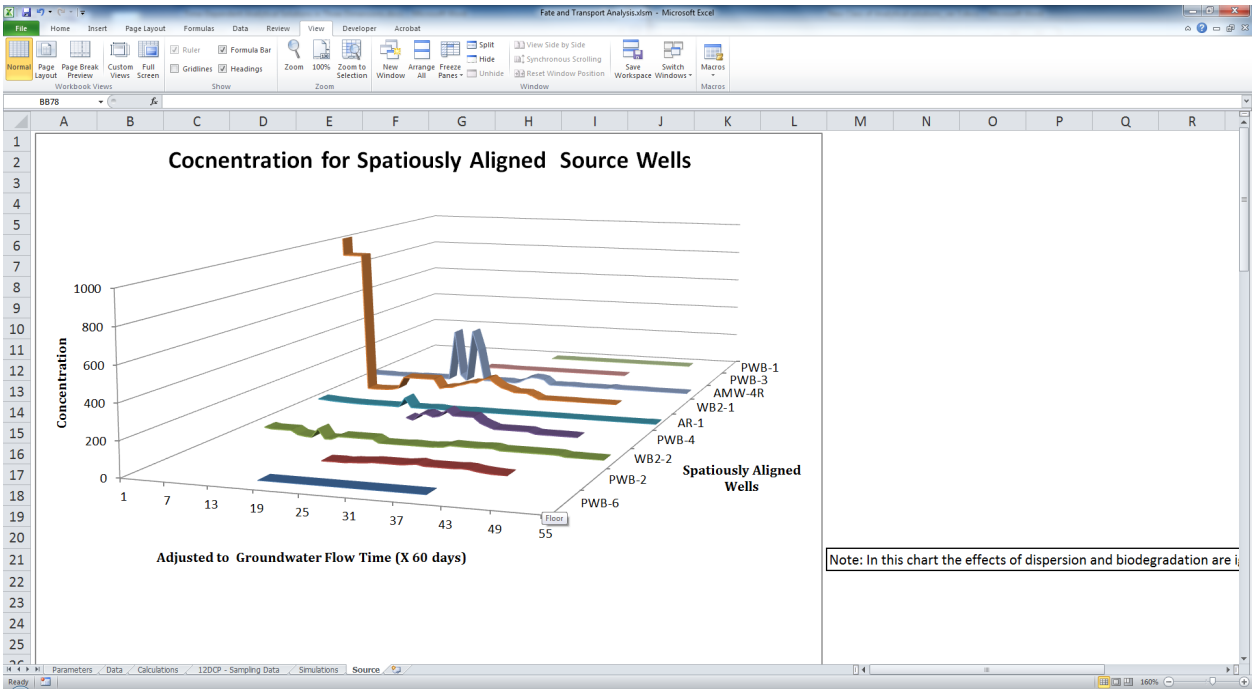


Fig.17. Fragment of the table on the same worksheet



	PWB-6			PWB-2			WB2-2			PWB-4			AR-1		WB2-1		
T0 - Xo/V	T0	T0 - Xo/V	C0	T0	T0 - Xo/V	C0	T0	T0 - Xo/V	C0	T0	T0 - Xo/V	C0	T0	C0	T0	T0 - Xo/V	C0
-36																	
-30																	
-24																	
-18															56	-15	1,700
-12															59	-12	890
-6																	890
0																	890
6																	890
12													5	18.0	84	13	5.00
18													6	16.0	91	20	3.00
24													41	12.0	99	28	4.00
30							56	31	**47.0**				44	10.00	112	41	5.00
36							59	34	**40.0**				47	8.00	118	47	8.00
42									**40.0**				52	6.00	126	55	18.0
48									**40.0**				56	5.00	132	61	93.0
54									**40.0**				59	4.00			93.0
60							84	59	**17.0**					4.00			93.0
66							91	66	**11.0**					4.00			93.0
72							99	74	**8.00**					4.00			93.0
78							112	87	**60.0**					4.00			93.0
84							118	93	4.00				84	4.00	156	85	34.0
90							126	101	5.00				91	3.00	160	89	44.0
96							132	107	**23.0**				99	62.0	164	93	47.0
102									**23.0**				112	3.00	168	97	62.0

Fig.18. The Close-up of the Graph on the same Worksheet



7 Concluding Remarks

This is not a fully developed software. One who decides to use it has to have a certain degree of understanding of its functional features and the analytical model that it uses. Assuming the user has gained this understanding, this software can serve him as a simple and, at the same time, very effective tool in practical analysis of on-going groundwater remedial investigation projects data, from sampling event to sampling event updating the data tables, adjusting the parameters and replotting the corresponding tables. With the use of Canvas or other commercially available software, one can create an animated 3D picture of the plume evolution that would contain all the information accumulated over the period of sampling activities. Below is given such an animated 3D plume evolution file for the data analyzed in this software (Just click on the link below to view the animation).

Fate and Transport (Animation)

APPENDIX

The Model Used in This Software

This software is based on the created by the author analytical model. Below is given a brief description of this model.

The model is based on the solution of the fate and transport equation in three dimensions with a pulse shaped constant rectangular boundary condition. This solution can be written as

$$C(t,x,y,z|L,M) = \frac{C_0}{4} x_D e^{2x_D v_{D_x}} \int_{P(t)}^{t} \frac{d\tau}{\tau^{3/2}} \exp\left(-\frac{x_D^2}{\tau} - (v_D\gamma)^2\tau\right) \left\{\operatorname{erfc}\left(\frac{y_D - L}{\sqrt{\tau}}\right) - \operatorname{erfc}\left(\frac{y_D + L}{\sqrt{\tau}}\right)\right\} \left\{\operatorname{erfc}\left(\frac{z_D - M}{\sqrt{\tau}}\right) - \operatorname{erfc}\left(\frac{z_D + M}{\sqrt{\tau}}\right)\right\}, \quad (1)$$

where the limits of integration change depending on the time t:

$$P(t) = \begin{cases} 0, & \text{for } t \le T \\ t - T, & \text{for } t \ge T. \end{cases} \quad (2)$$

In the solution (1), L and M are dimensions of the patch, $x_D, y_D$and z_D are the rescaled by the corresponding dispersion coefficients x, y, z coordinates: $x_D = x/(2D_x)$, $y_D = y/(2D_y)$ and $z_D = z/(2D_z)$.

This solution was derived in [1], but is difficult to use since the integral it contains cannot be taken analytically. The author superimposed this solutions for each source well, thus forming a solution spatially varying transient source. This solution can be written as

$$C(t,x,y,z) = \sum_{i,j} C\left(t_j, x - x_0^{(i)}, y - y_0^{(i)}, z - z_0^{(i)} | L^{(i)}, M^{(i)}\right)$$

where $x_0^{(i)}, y_0^{(i)}, z_0^{(i)}$ are the x, y, z coordinate for the i-th source well, $L^{(i)}, M^{(i)}$ are corresponding dimensions of the patch for that well, t_j is the time at which a given data sample was taken. This formula forms the basis of the calculations in the software.

References

[1] F.J.Leij, T.H,.Skaggs, M.Th. van Genuchten. Analytical Solutions for Solute Transport in Three-Dimensional Semi-Infinite Porous Media, Water Resources Research, vol.27, No, 10 , 2719-2733, 1991.