Horizontal Plane Solution Model

Software for the Calculation of
Groundwater Contamination
Using the Horizontal Plane Solution

Version 1.0

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1.0 Introduction

The need to either predict the extent of groundwater contamination from a potential source or delineate the extent of existing groundwater contamination from a known source are common and useful hydrogeological exercises needed to address regulatory requirements or aid in remedial efforts. There are different tools that can be applied that vary from simple analytical models to complex numerical models depending on the contaminant, subsurface conditions and modeling goals.

Analytical models which are generally based on solving a single equation are easier to use but also have a greater number of assumptions and limitations with the need for careful use and consideration of the predictive results. Complex numerical models generally require greater time and expertise to construct but have fewer assumptions and limitations with better predictive results for complex environments. Both can be affected by the quality of data inputs which reflect the subsurface and contaminant characteristics.

2.0 Models

2.1 DEQ Domenico Model

One of the most common analytical solutions for groundwater contaminant flow is the Dominico model (Domenico and Robbins, 1985; Domenico, 1987). The Domenico solution solves for a three-dimensional differential equation for solute transport in a saturated porous medium with uniform steady-state flow, one dimensional advection, three-dimensional dispersion, adsorption and first order decay. The Domenico solution has relatively simple mathematical expressions that are easy to implement and readily allow modifications of boundary conditions.

The Domenico solution has been shown to introduce errors under certain conditions (Guyonnet & Neville, 2004; Srinivasan et al, 2007; West et al, 2007) because of the approximate analytical solution and underlying assumptions. The Domenico solution also employs a vertical plane source (Figure1). In order to use a vertical plane source solution for a horizontal plane source, a mixing zone is generally

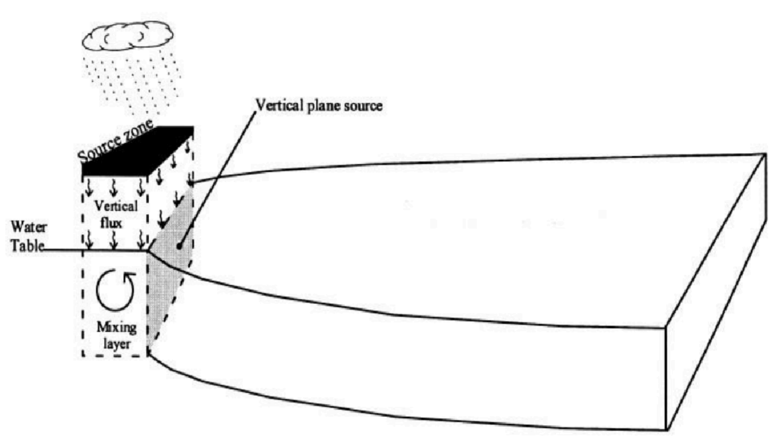

Figure 1. Vertical plane source used in the Domenico solution (Tonsberg, 2014).

used. The mixing zone assumes instantaneous mixing of a unit volume of contaminant and ground water based on infiltration and flow rates respectively along with a user specified depth. The estimate of the mixing zone depth and assumption of instantaneous mixing can result in additional errors.

2.2 Horizontal Plane Solution

The horizontal plane source (HPS) model as applied to contaminant transport is described in Galya (1987). The HPS solution also solves for a three-dimensional differential equation for solute transport in a saturated porous medium with uniform steady-state flow, one dimensional advection, three-dimensional dispersion, adsorption and first order decay. The HPS model is a three-dimensional analytical solution developed using Green's functions for an aquifer with uniform physical properties, a horizontal plane source and an input mass source rate. The mathematical development of the HPS is well described in Carslaw & Jaeger (1959), Galya (2004) and Tonsberg (2014).

The HPS model described by Galya (1987) is capable of including multiple sources with varying dimensions and source concentrations that can vary with time. Galya (1987) presents a Fortran code that derives the solution by numerical integration over the time period of interest using the trapezoidal rule. Because the HPS model incorporates a horizontal plane source, a calculated mixing zone depth and mixed source concentration utilized in the Domenico model is not needed.

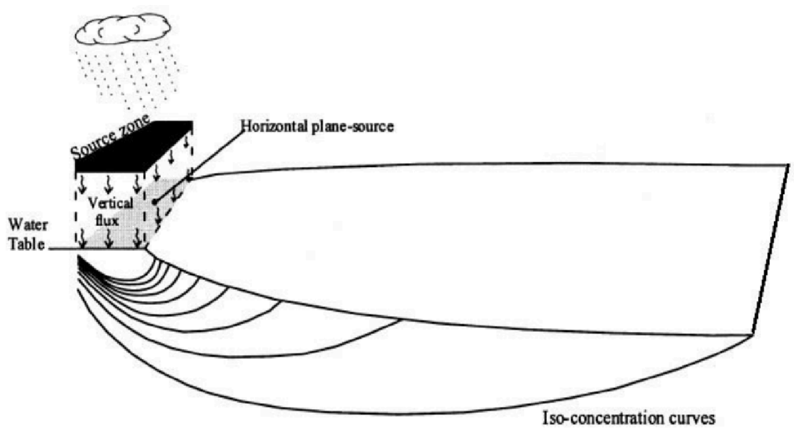

Figure 2. Horizontal plane source (Tonsberg, 2014).

3.0 HPS Model Installation

The HPS model, Python and Fortran source codes, executable, image files and documentation can be downloaded from the Github repository (https://github.com/GWModels/HPS-Model). The folder with the executable and image files should be unzipped and retained in a single folder. The executable along with the associated files should be run within the folder. When executed certain output files, described below, will be created every time the model is run and placed in the same folder. A pdf and GeoTIFF of model results can also be saved with the user preferred name and location. The HPS model software is being provided under a GNU General Public License Version 3.0.

4.0 HPS Python/Fortran 90 Model Description

4.1 General

This HPS Python/Fortran 90 model is composed of a pre- and post-processor written in Python 3.12 and a Fortran 90 program that solves for groundwater concentrations. A Fortran based program was retained for calculating groundwater concentrations because of its ability to efficiently handle the highly iterative nature of the solution and large number of computations required, which allows for timely execution and results. The Fortran program created by Gayla (1987) was written in Fortran 77 and solved for a limited number of individual observation points. The original Fortran program by Gayla (1987) was rewritten and compiled in Fortran 90 and edited to solve for a large number of contiguous observation points that represents an area specified by the user which could then be easily mapped and contoured. The original Fortran program also utilized text-based input and output files. The Python pre-processor allows for easier entry and creation of input data for each model scenario that is passed to and utilized by the Fortran program. The Python post-processor consists of two parts (1) display of input and output data along with a contour map of groundwater concentrations and (2) links to create a pdf file of the displayed results and creation of a contoured groundwater concentration GeoTIFF file that can be used as input to Geographical Information Systems software.

A number of Python libraries were utilized in the pre- and post-processors. Tkinter, Matlibplot and Scipy were used for the data entry and display along with creation of the groundwater concentration contour map. Math, Numpy and Pandas were used for various calculations and array creation. Fpdf was used for the pdf file creation and Rasterio for creation of the GeoTIFF. F2py, which is part of the Numpy library, was used to create a Fortran wrapper function for the Fortran program that could be called by Python.

4.2 Model Input

Data input for a model scenario is entered in the Input tab of HPS model. The Input tab prompts the user for the necessary data to run the model with up to five (5) sources and five (5) specific observation points (Figure 3). The input data is divided into four sections (1) aquifer parameters, (2) model parameters, (3) source characteristics, (4) observation point locations. The units of input data are indicated adjacent to the entry cell. After the input data has been entered, clicking on the "Run Model" button will run the model with the current input values.

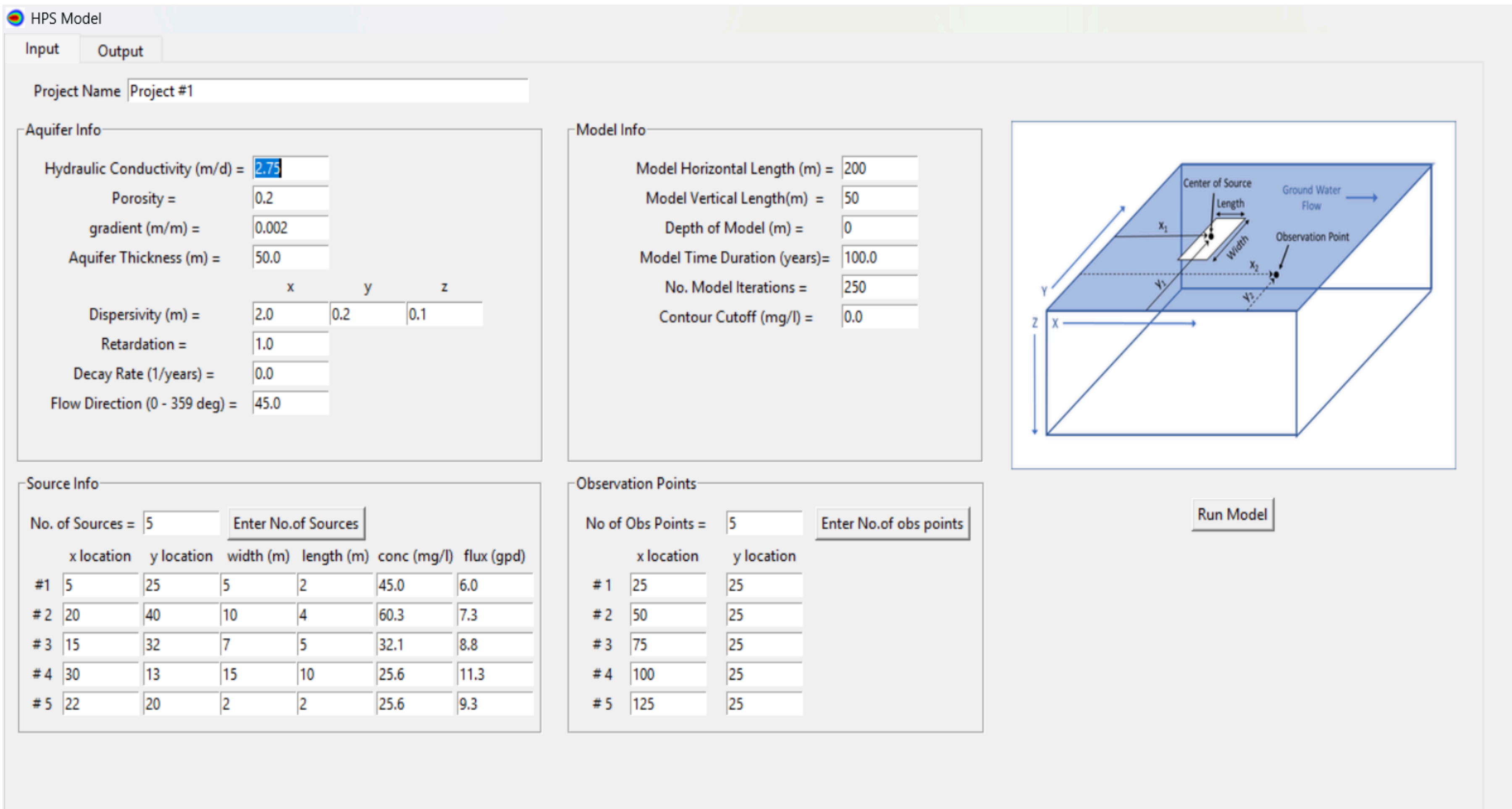

Figure 3. HPS model input screen.

4.2.1 Aquifer Parameters

- Hydraulic Conductivity. The units of hydraulic conductivity are in meters per day. There is no anisotropy considered.
- Porosity. The porosity is an effective porosity.
- Gradient. The slope of the groundwater surface.
- Aquifer Thickness. The units of thickness of the aquifer are in meters. The thickness of the aquifer is the measure from the base of the aquifer to the top of the water table.
- Dispersivity. Dispersivity is a characteristic of the aquifer that causes the spreading of a contaminant in the longitudinal, transverse and vertical directions downgradient from the source. The units of dispersivity are in meters.
- Retardation. Retardation describes the slower velocity of solutes compared to the velocity of the groundwater. The numerical value expresses the ratio of groundwater velocity divided by the contaminant velocity. The number one (1) would represent no retardation and numbers greater than one (1) would represent some value of retardation.
- Decay Rate. The decay rate expresses the rate at which a contaminant within the groundwater decreases in concentration over time due to abiotic and biotic processes. The decay rate represents a first order decay coefficient defined by 0.693 / [half-life in years] with units of 1/years.
- Flow Direction. The groundwater flow direction is the direction described in degrees from 0 to 359. The flow direction is used in creating the GeoTIFF file that can be imported to GIS software.

All location data are in meters entered as whole numbers. The number of sources or observation points can be added or removed by changing the number of each then clicking the “Enter No. of Sources” or “No. of Obs Pts” buttons. Rows will be added or removed from the last row.

4.2.2 Model Info

- Model Horizontal Length. The length of the model in whole meters along the downgradient (x) direction. The origin of the model length is always zero (0) in relation to the source location. Shorter model lengths may terminate the model results prior to the entire plume extent and only shows a portion of the groundwater contamination (Figure 4).
- Model Vertical Length. The length of the model in whole meters along the cross gradient (y) direction. The origin of the model length is always zero (0) in relation to the source location. Shorter model lengths may terminate the model results prior to the entire plume extent and only show a portion of the groundwater contamination (Figure 4).
- Depth of Model. The depth below the ground water surface in whole meters of model calculations defined by a plane with x and y limits defined by the model horizontal length and model vertical length.
- Model Time Duration. A specified time period in years for the model calculations.

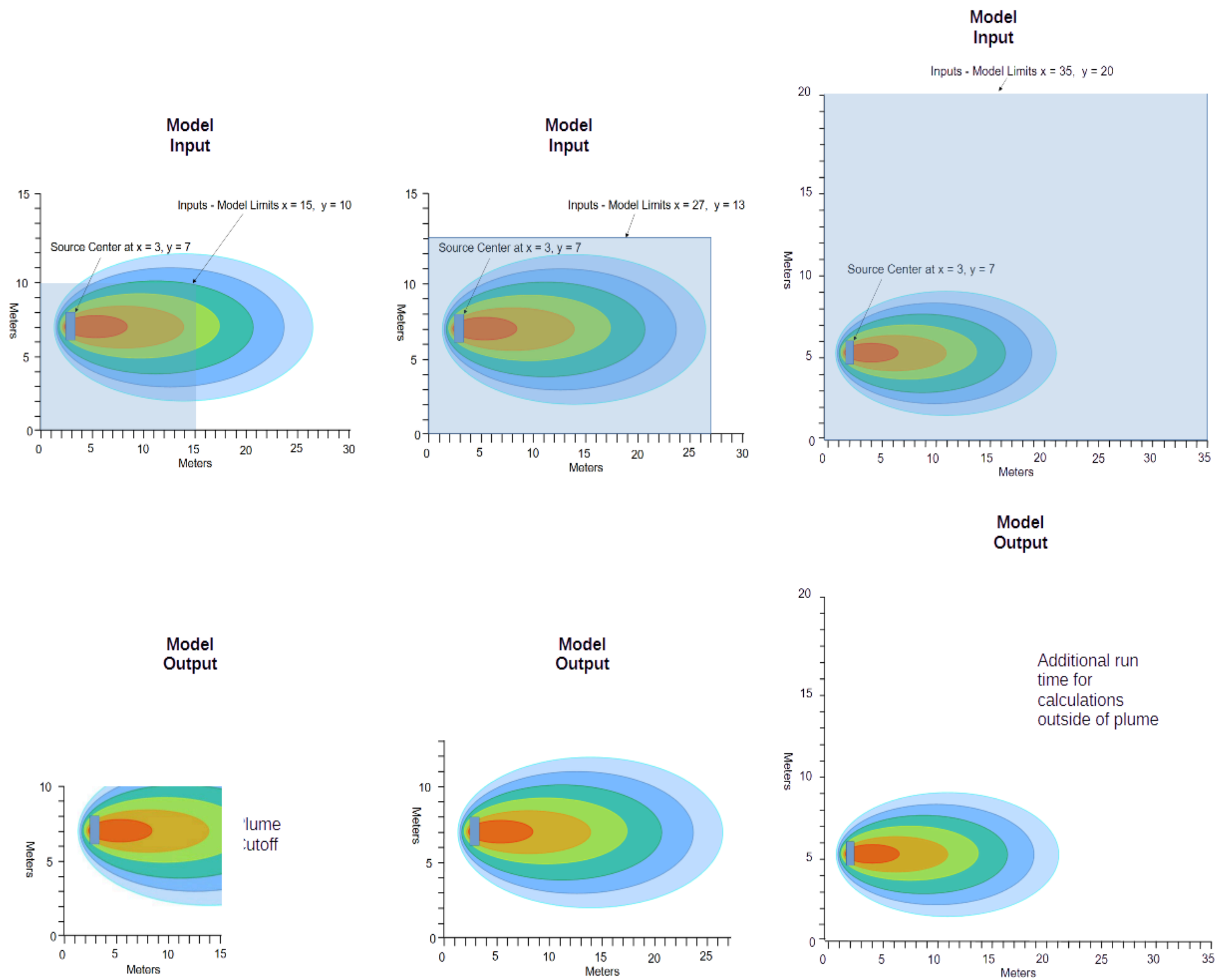

Figure 4. Model limits and output

- No. of Model Iterations. The model utilizes trapezoidal numerical integration to solve for the groundwater contaminant concentrations. The approximate solution is achieved by algebraic summation of a number of smaller trapezoids to calculate the area under the curve. The size of each trapezoid is defined by the number of model iterations. The greater the number of iterations the smaller is each numerical part and the more accurate the answer. Conversely the greater the number of model iterations the greater the computation time.
- Contour Cutoff. The HPS model will calculate for every x and y combination as defined by the model horizontal length and model vertical length that can extend beyond the dimensions of the plume. It may be beneficial to restrict the display of the plume extent as defined by a regulatory limit or minimum contaminant level. The model should be run with the contour cutoff set to zero (0) until a final solution is achieved. An appropriate contour cutoff can be determined and will display only values greater than the contour cutoff in the output tab along with the pdf and GeoTIFF files (Figure 5).

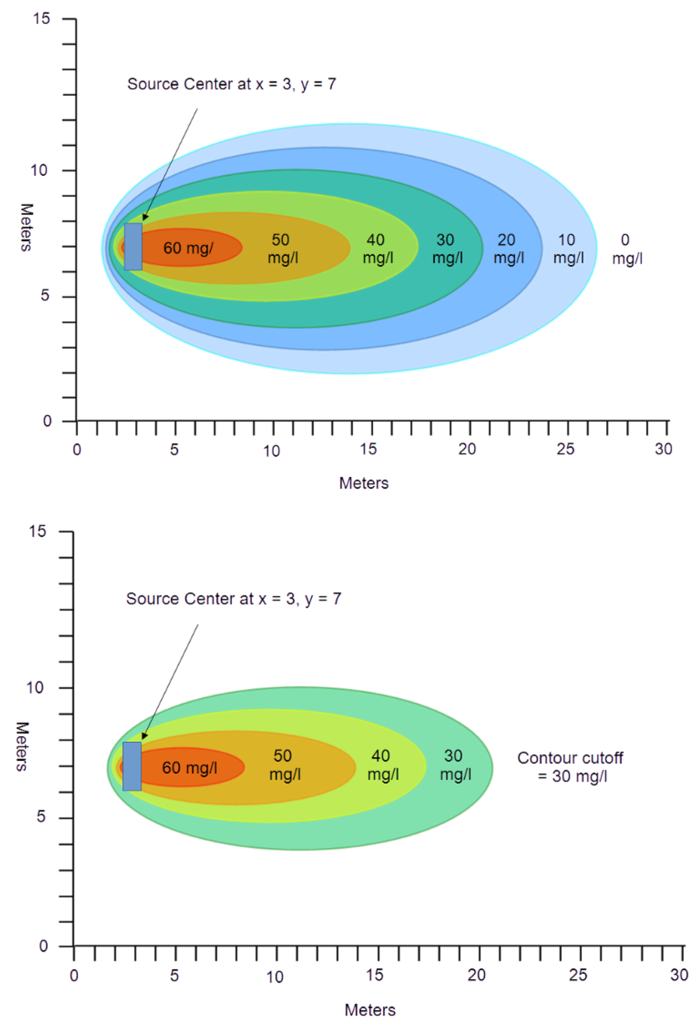

Figure 5. Contour cutoff

4.2.3 Source Info

- No. of Sources. The number of different sources for the model scenario with unique characteristics for each defined below. No more than five (5) sources can be entered.
- X Location. The length in the downgradient direction (x axes) in whole meters from the origin to the center of the source (Figure 6).
- Y Location. The length in the cross gradient direction (y axes) in whole meters from the origin to the center of the source (Figure 6).
- Width. The dimension of the source in whole meters that is perpendicular to the flow direction (y axes) (Figure 6).
- Length. The dimension of the source in whole meters that is parallel to the flow direction (x axes) (Figure 6).
- Concentration. The concentration of the source in milligrams per liter that is a constant throughout the source area and over the model duration.
- Flux. The rate of contaminant flow in gallons per day that is a constant throughout the source area and over the model duration.

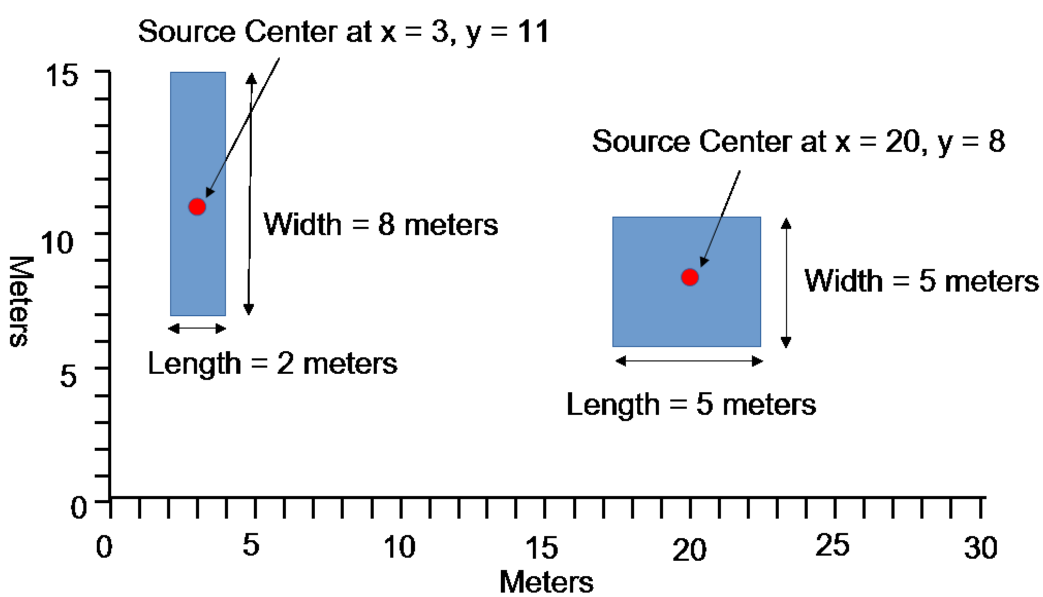

Figure 6. Source location and dimensions

4.2.4 Observation Point Info

- No. of Observation Points. The number of different observation points for the model scenario with unique locations for each defined below. No more than five (5) observation points can be entered.
- X Location. The length in the downgradient direction (x axes) in whole meters from the origin to the observation point.
- Y Location. The length in the cross gradient direction (y axes) in whole meters from the origin to the observation point.

  The depth of the observation point is the same as the depth of the model.

The location of observation points must be within the model boundary limits as described in Section 4.2.2.

4.3 Model Output

The model output can be viewed in the output tab after the model has been run. The output data is divided into four sections (1) concentration contour map, (2) table description of the model input data, (3) table of source and observation point data, (4) pdf and GeoTIFF output

4.3.1 Concentration Contour Map. The concentration contour map shows the concentration contours of the model scenario with ten (10) contour intervals (Figure 7). The map also shows the center location and

identifying numbers of all the sources along with the location and identifying numbers of all the observation points. The identifying numbers used in the contour map match the numbers used in the table descriptions. The length of the x and y axis reflect the model dimensions as described on the input tab. **The x and y axis of the contour map are not to scale**, but were sized to fit onto the page.

4.3.2 Table of Model Input Data. The table provides a description of the input data used for concentration results and creation of the contour map.

4.3.3 Table of Source and Observation Point Data. The table provides a description of the source information that includes location, concentration and flux rate. The table also describes the location and groundwater contaminant concentrations at the observation points. The identifying number of the source and observation points match the identifying numbers as seen on the contour map.

4.3.3 Pdf and GeoTIFF Output. There are two (2) buttons included in the output page. One for generation of a pdf file and another for the generation of a GeoTIFF file. Clicking the “Export pdf” button will launch a window that prompts the user for a file location and name. The pdf generated will contain all the information presented in the output tab (Attachment 1.). Clicking on the “export GeoTIFF" button will also launch a window that prompts the user for a file location and name. The resulting file is a GeoTIFF of the contour map as seen in the output tab (Figure 8). The GeoTIFF is referenced by entering the Universal Transverse Mercator (UTM) coordinates of Source #1 in the boxes below the button. The orientation of the contaminant plume is defined by the “Flow Direction” as defined in the input tab.

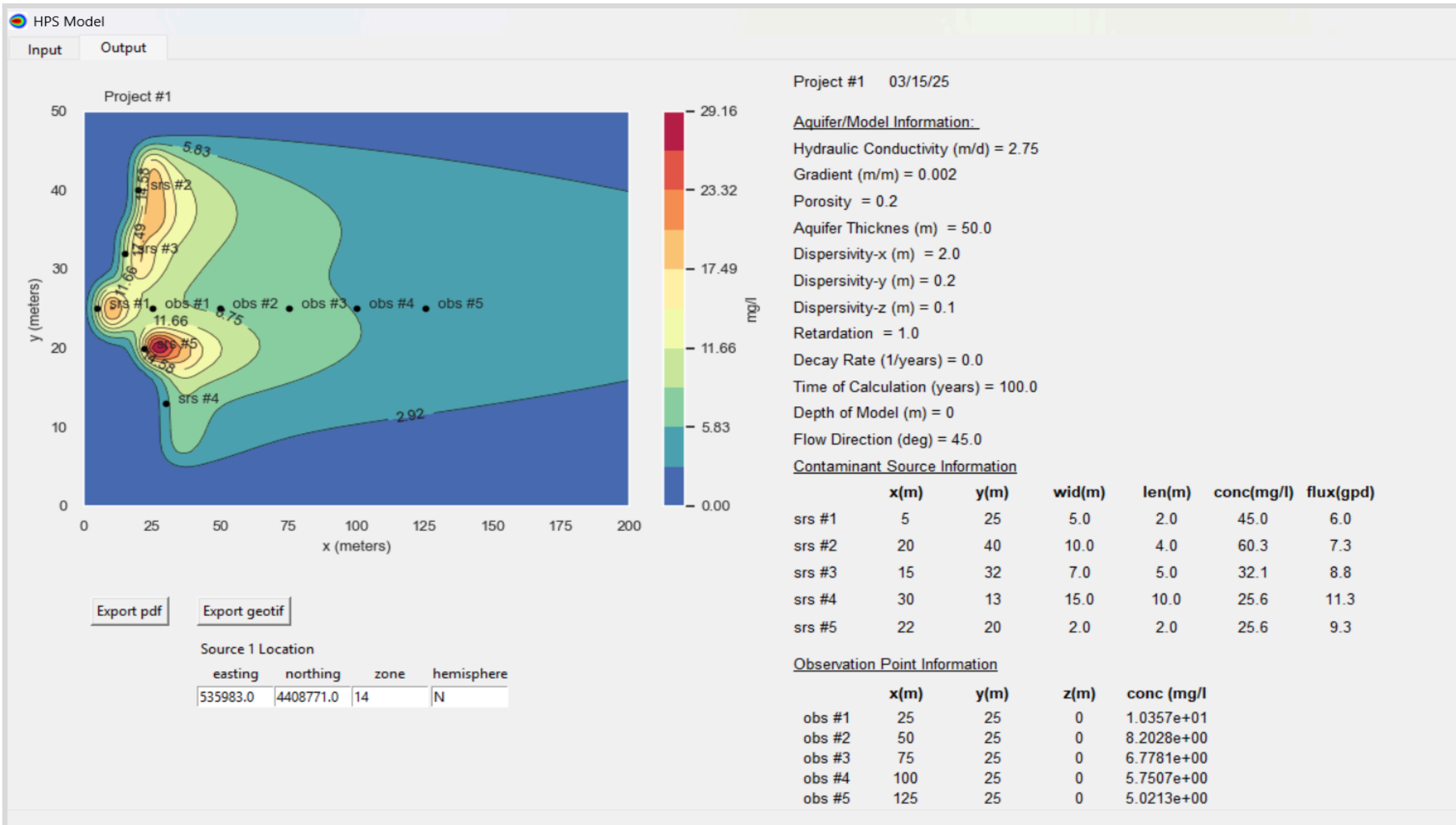

Figure 7. HPS model output screen.

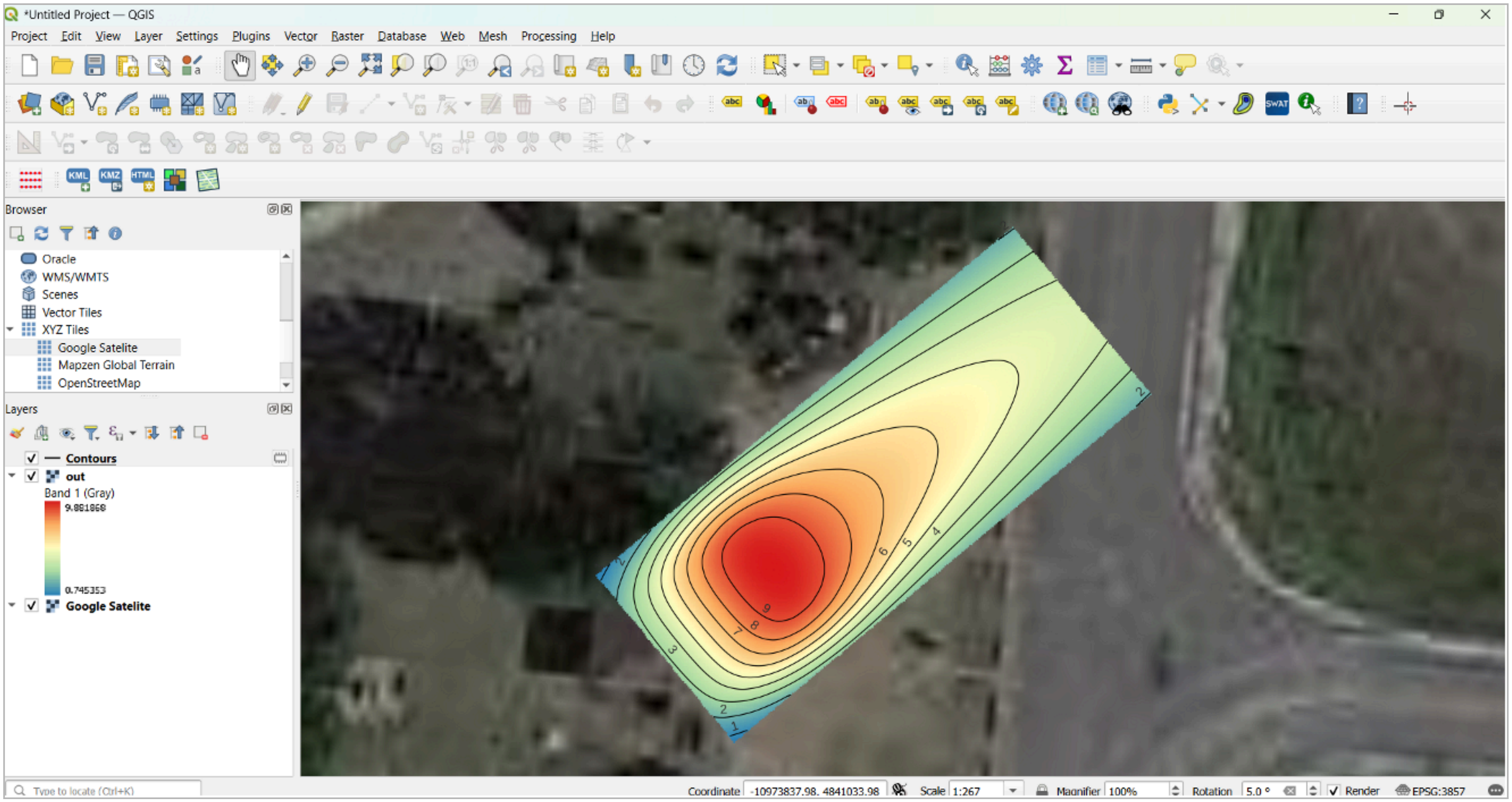

Figure 8. Imported HPS GeoTiff with added color map and contours in QGIS.

The rest of the model results will be rotated around the source #1 location. The resulting GeoTIFF can be imported to commonly used Geographical Information System (GIS) software.

In addition every time a contour map is generated in the output tab a text file is generated (hps_xyz.csv) in the parent directory that includes the x, y locations in model coordinates and corresponding concentration data. If a GeoTIFF is created another text file will be generated i(hps_utm.csv) n the parent directory with the rotated x, y locations in UTM coordinates along with the corresponding concentration data. The text files can also be imported to GIS or other contouring software.

5.0 HPS Python/Fortran 90 Model vs Fortran (Gayla, 1987) Program

The HPS model was incorporated into a Python/Fortran 90 program based on the Fortran code presented in Galya (1987). The implementation of the HPS solution using a Python pre- and post processor results in a much easier to use tool than a compiled Fortran program with textural inputs and outputs. The graphical abilities of Python are useful for viewing and interpreting results.

The Fortran program code was compiled using Code::Blocks (2021) and the GNU Fortran compiler (2021). The original program was written in Fortran 77 and code modifications were made to be compliant with Fortran 90 so that it could be compiled with a modern compiler.

Confirmation of the HPS Python/Fortran 90 model results was accomplished by comparison of the results from the Fortran code as described in Galya (1987). The model scenario used for comparison was for a single source with the size, contaminant and aquifer characteristics described in Table 1. The results of the simulation were calculated along various points along the plume center line (Y = 0) and at the aquifer surface (Z = 0). The model scenario results for the HPS Python/Fortran 90 model and the Gayla Fortran program can be seen in Table 2 and Figure 9 and 10 below.

Table 1. Model Scenario Characteristics

Drainfield	
Width (meters)	80
Length (meters)	12
Concentration (mg/l)	45
Recharge Rate (meters/day)	6.34E-05
Hydraulic Conductivity (meters/day)	2.75
Groundwater Velocity (meters/day)	0.027
Hydraulic Gradient (meters/meter)	0.002
Porosity	0.2
Aquifer Thickness (meters)	50
Dispersivity	
Longitudinal (meters)	2
Transverse (meters)	0.2
Vertical (meters)	0.2
Retardation	1
Decay (1/Year)	0
Source Location	
X	0
Y	0
Z	0

Table 2. HPS Python/Fortran Model vs. Fortran program model results

X Location (meters)	HPS Python/Fortran Model (mg/l)	HPS Fortran Program (Gayla,1987) (mg/l)
100	0.78	0.78
200	0.55	0.56
300	0.45	0.45
400	0.39	0.39
500	0.35	0.35

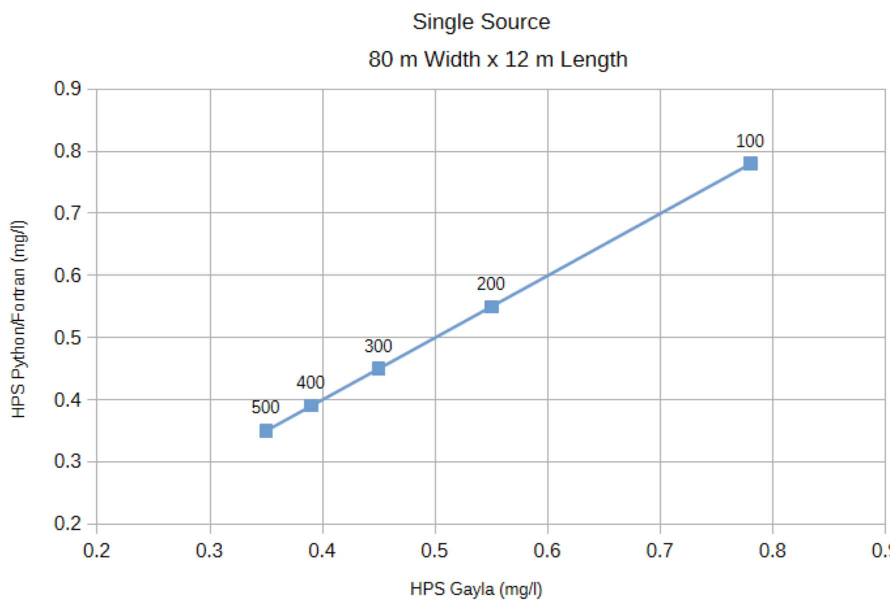

Figure 9. HPS Python/Fortran 90 vs. Fortran (Gayla, 1987) program model results at downgradient locations along the plume centerline as measured in meters.

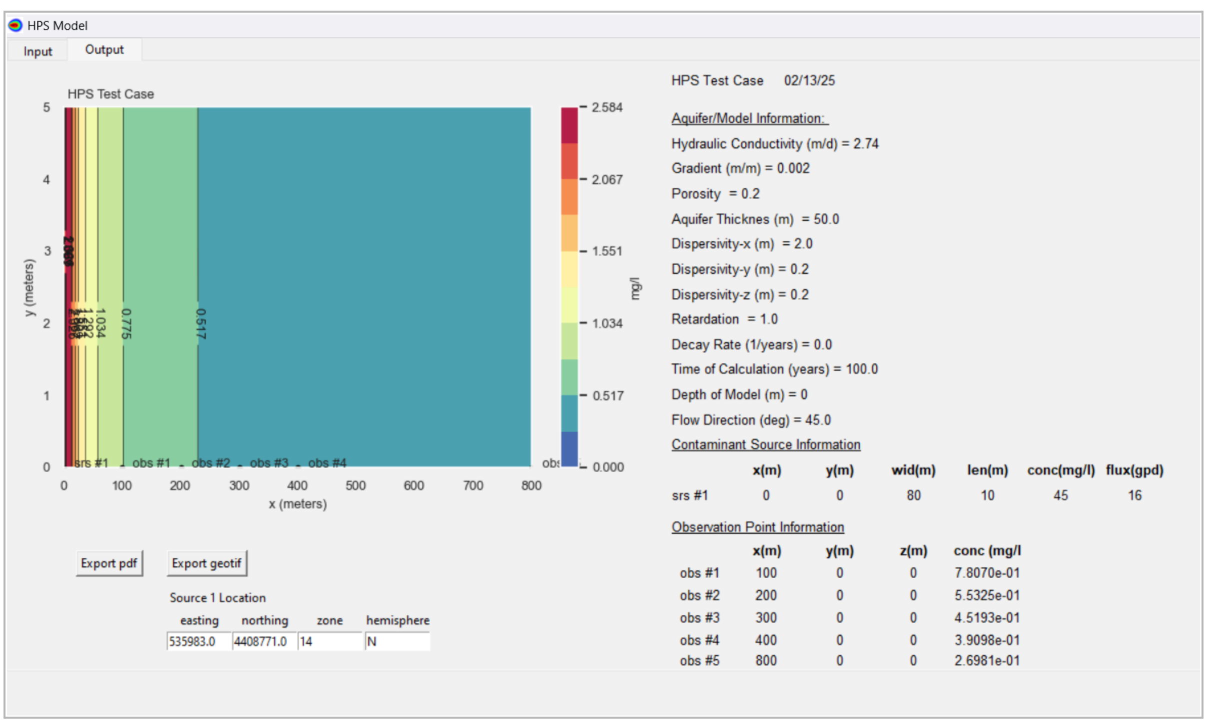

Figure 10. HPS Python/Fortran model results at downgradient locations along the plume centerline as measured in meters.

6.0 HPS Python/Fortran 90 Model vs Numerical Model

6.1 Modflow Model Construction

Additional corroboration was completed by comparing the HPS Python/Fortran 90 model results with a Modflow numerical model. The model was constructed using the U.S. Geological Survey's graphical user interface ModelMuse -Ver 4.3.0.0 (USGS, 2020) and Modflow 2005 (USGS, 2019) with the inputs described in Table 1. The Modflow model is 1,000 meters in length, 500 meters in width and 50 meters in depth. The model was constructed with a variable density grid with finer grid spacing in the vicinity of the drainfield(s) and coarser farther down gradient (Figure 4). The upgradient and downgradient boundaries were defined with constant head nodes of 0 meters and -2 meters respectively. Lateral boundaries were defined as no-flow or impermeable boundaries. Longitudinal, transverse and vertical dispersivity values were 2.0, 0.2 and 0.2 meters respectively. The model was run as a transient model with a time frame of 100 years divided into 87 stress periods.

6.2 Single Contaminant Source

The single source has the same dimensions as the example presented in Gayla (1987) with a width of 80 meters and a length of 12 meters. The recharge area of the source was a rate of 7.57E-5 meters per day and a contaminant concentration of 45 milligrams per liter. The Modflow construction and source location can be seen in Figure 11. The results of the Modflow model were very similar to the HPS Python/Fortran model and can be seen in Table 3 and Figures 12 and 13. Differences were most likely due to grid spacing and numerical dispersion. The nearly identical values indicate that the HPS Python/Fortran model produces predictive results that are comparable to a numerical model with the scenario described in Table 1.

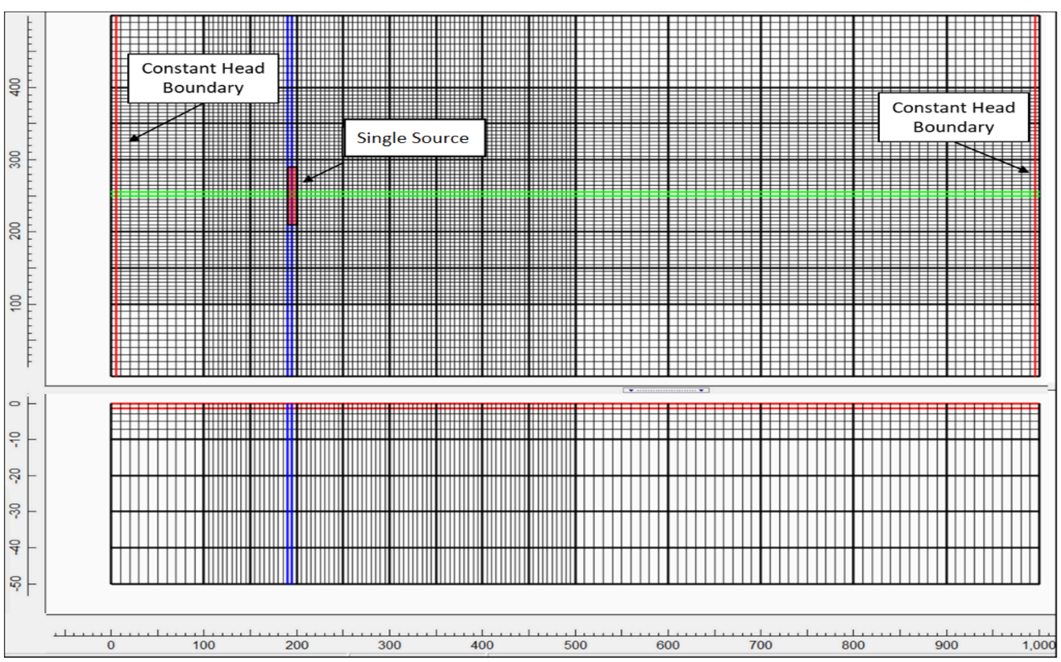

Figure 11. Plan view (upper) and cross-sectional view (lower) of Modflow model construction for one source comparison with HPS Python/Fortran model results. Axes are in meters

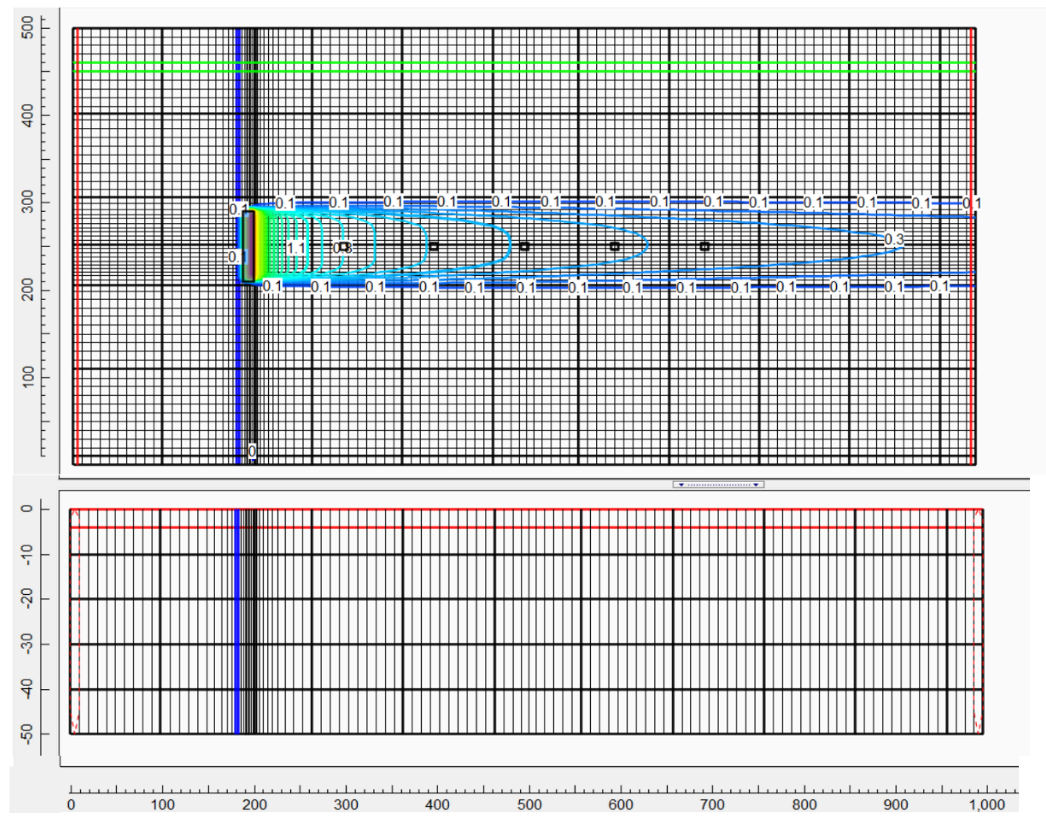

Figure 12. Plan view (upper) and cross-sectional view (lower) of Modflow single source model results. Axes are in meters and concentrations are in milligrams per liter (grams/meter^3).

Table 3. Single Source HPS spreadsheet vs. Modflow model results

X Location (meters)	HPS Python/Fortran 90 Model (mg/l)	Modflow (mg/l)
100	0.78	0.78
200	0.55	0.56
300	0.45	0.47
400	0.39	0.40
500	0.35	0.36

Rooted mean square residual = 0.012 mg/l

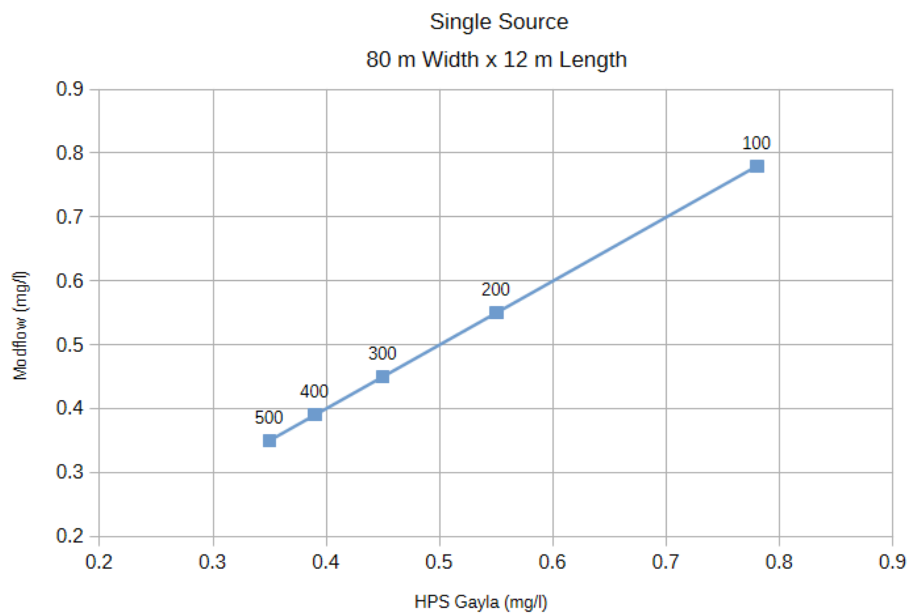

Figure 13. HPS Python/Fortran vs. Modflow model results at downgradient locations along the plume centerline as measured in meters

6.3 Two Contaminant Sources

The HPS Python/Fortran model was also compared to the results of a Modflow numerical model with two separate sources with overlapping contaminant plumes. The Modflow construction was identical to the single source model. Two sources with dimensions of 30 meters in width and 10 meters in length were placed with the Source 1 center location at x = 5 meters and y = 45 meters and Source 2 at x = 55 meters and y = 65 meters respectively. The recharge area of the source was a rate of 7.57E-5 meters per day and a contaminant concentration of 45 milligrams per liter. The Modflow construction and source location can be seen in Figures 14. The results of the Modflow model were very similar to the HPS Python/Fortran model and can be seen in Table 4 and Figures 15 and 16.

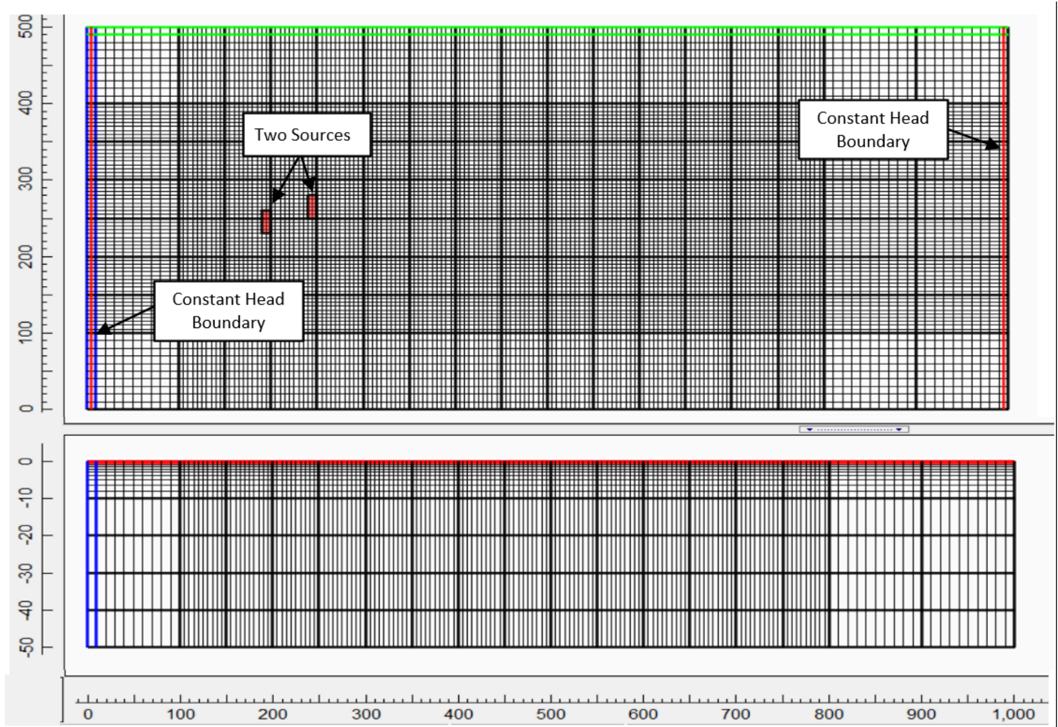

Figure 14. Plan view (upper) and cross-sectional view (lower) of Modflow model construction for two source comparison with HPS Python/Fortran model results. Axes are in meters

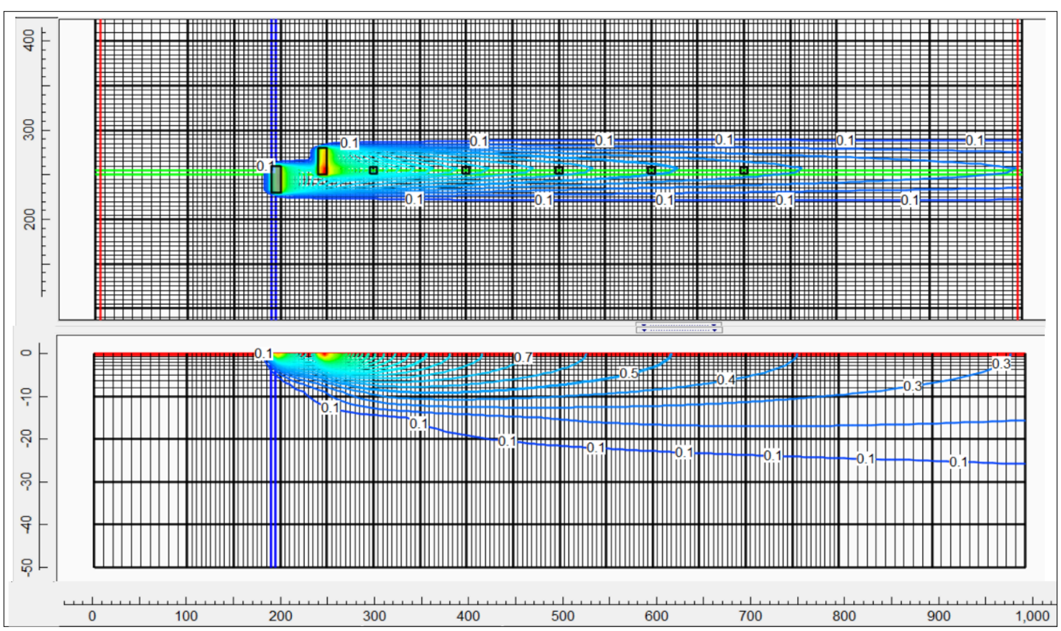

Figure 15. Plan view (upper) and cross-sectional view (lower) of Modflow two source model results. Axes are in meters and concentrations are in milligrams per liter (grams/meter^3).

Table 4. Two Source HPS spreadsheet vs. Modflow model results

X Location (meters)	HPS Python/Fortran 90 Model (mg/l)	Modflow (mg/l)
100	1.49	1.45
200	0.85	0.86
300	0.63	0.65
400	0.51	0.52
500	0.43	0.44

Rooted mean square residual = 0.022 mg/l

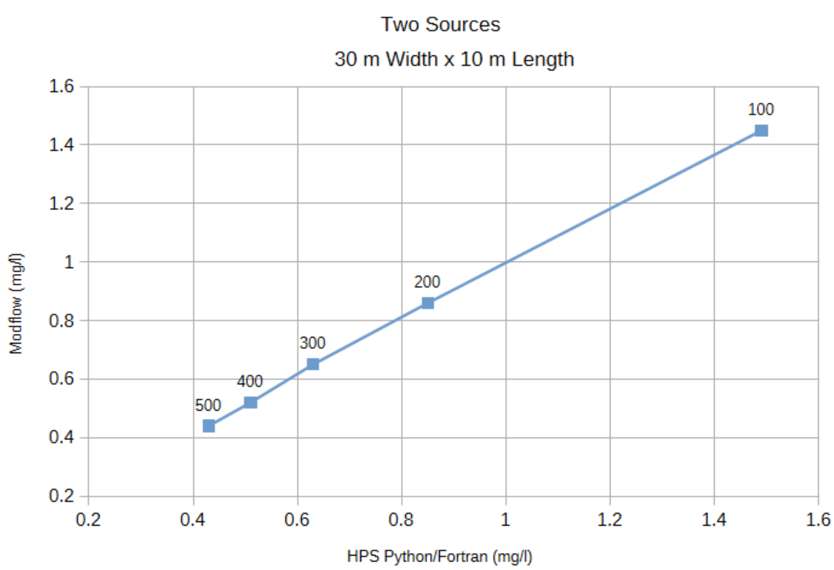

Figure 16. HPS Python/Fortran vs. Modflow model results at downgradient locations along the plume centerline as measured in meters

7.0 Conclusion

The HPS Python/Fortran 90 model appears to provide accurate predictive downgradient concentrations for simple hydrogeologic systems. The use of a Python preprocessor makes the entering of model data easier and the post processor provides needed text and contaminant map in a consolidated format for review. Retaining the original Fortran code with some modifications provides for computational efficiency with shorter run times.

8.0 Disclaimer & Limits of Liability

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Attachment 1. HPS model pdf output

HPS Model Results

Project Name 04/04/25

Aquifer/Model Information:

Hydraulic Conductivity (m/d) = 2.75
Gradient (m/m) = 0.002
Aquifer Thicknes (m) = 50.0
Dispersivity-x (m) = 2.0
Dispersivity-y (m) = 0.2
Dispersivity-z (m) = 0.1
Retardation = 1.0
Decay Rate (1/years) = 0.0
Time of Calculation (years) = 100.0
Depth of Model (m) = 0
Flow Direction (deg) = 45.0

Contaminant Source Information

	x(m)	y(m)	wid(m)	len(m)	conc(mg/l)	flux (gpd)
srs #1	2	6	10.0	1.0	45.0	5.0

Observation Point Information

	x(m)	y(m)	z(m)	conc(mg/l)
obs #1	10.0	6.0	0.0	9.272155e+00
obs #2	15.0	6.0	0.0	7.052690e+00

HPS Model Results