

## GIS-based Contaminant Transport Model for Heterogeneous Hydrogeological Settings

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**ABSTRACT.** The development and implementation of a GIS-based Contaminant Transport Model (GIS-CONTRAM) is herein described. GIS-CONTRAM can be employed to model fate and transport of contaminants in the subsurface. ArcGIS' ModelBuilder and Visual Basic (VB) Scripts are used in 3 integrated steps, to enable GIS-CONTRAM to accommodate spatial variabilities in hydrogeological parameters without compromising computational efficiency. The new model can be easily coupled with vadose zone contaminant transport models. Visual MODFLOW was used for validation of GIS-CONTRAM. Comparisons of configurations and results of GIS-CONTRAM with those of Visual MODFLOW, which is widely used to model groundwater flow and contaminant transport, indicate reasonable correlation with  $R^2$  values of 0.63 and 0.95 for synthetically generated heterogeneous and homogeneous hydrogeological conditions, respectively. Thus, although not as comprehensive as Visual MODFLOW, GIS-CONTRAM provides reasonable contaminant transport results.

*Keywords:* GIS, groundwater, contaminant fate and transport, model, Visual MODFLOW

### 1. Introduction

There are several sources of groundwater contamination, including tanks, septic systems, hazardous waste sites, landfills, and mining sites. In the U.S. Environmental Protection Agency (USEPA)'s National Priority List, 78% of sites have some form of groundwater contamination. Mitigation of the impacts of groundwater contamination depends on the understanding and modeling of contaminant transport and fate in the groundwater. Modeling contaminant fate and transport in groundwater usually involves the use of one of several available solutions of the advection-dispersion equation (ADE), with assumptions of various boundary conditions (Domenico and Schwartz, 1990).

However, most solutions assume constant hydrogeological conditions, and as discussed by Grathwohl and Kleinedam (1995) and Fuller et al. (1996), homogeneous soils and constant groundwater flow are not very common. Spatial variabilities can be very significant. In turn, they affect contaminant transport mechanisms and rates. If spatial variability of the transport medium is considered, transport equations can develop into very complex mathematical expressions, as evident in analyses by Bai et al. (1996, 1997), making it necessary to use computer models that can discretize the subsurface system into

Finite Element meshes. There are several types of software in the market that combined, can model groundwater flow and contaminant transport. Among them are the widely used U.S. Geological Survey Modular Groundwater Model—MODFLOW (Hill et al., 2000), RT3D (Clement et al., 1998) and/or MT3DMS (Zheng and Wang, 1999), which when combined, can be used to model contaminant transport in the subsurface.

The complexities of applying existing contaminant transport models to highly heterogeneous sites, often constrains the use of such models to experts in the area. The motivation behind GIS-CONTRAM is to provide an easy-to-use model that can be incorporated to other risk assessment models by users at various levels of expertise, while accommodating such heterogeneity. For this reason, a semi-analytical Geographic Information Systems (GIS)-based solution to the ADE, is developed and customized for the assessment of contaminant transport and fate in groundwater. Semi-analytical term is used because the methodology is not a straightforward application of an analytical solution. Instead, it uses a combination of spatial tools of ArcGIS to incorporate changes to groundwater direction and geological properties to an analytical solution. The model is built into GIS, which is widely used by environmental science professionals, will allow time/cost-effective assessments of contaminant transport in the subsurface under very variable conditions. It can be easily integrated with other GIS-based environmental assessment models such as HAZUS-MH developed by the Federal Emergency Management Agency (FEMA, 2003). The creation and use of the GIS-based Contaminant Transport Model (GIS-CONTRAM) makes it unnecessary to depend on non-GIS tools for assessments for

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contaminant transport in heterogeneous subsurface.

## 2. Approach to GIS-CONTRAM Development

### 2.1. Contaminant Transport Mechanisms

There are three major processes that should be considered when developing a contaminant transport model: advection (convection), dispersion and diffusion (Figure 1). However, molecular diffusion is only significant when the contaminant is traveling through fine-grained soils, with hydraulic conductivity below  $1.6 \times 10^{-8}$  cm/s (Gillham and Cherry, 1982). Such low conductivities are not easily found in aquifer materials (Batu, 2006). Therefore, molecular diffusion can be assumed to be negligible when modeling contaminant transport in groundwater and will not be considered herein.

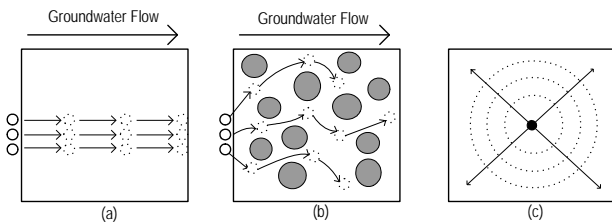


Figure 1. Subsurface contaminant transport components: (a) convective transport; (b) mechanical dispersion; and (c) diffusion.

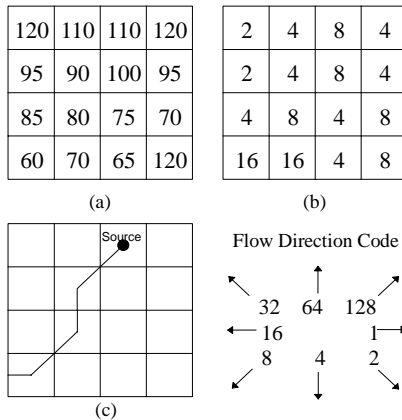


Figure 2. GIS flow direction determination steps: (a) interpolate cell elevation from monitoring wells; (b) code for preferred flow direction from each cell; and (c) flow path from a source point.

### 2.2. Approach to Determination of Groundwater Flow Direction

An important aspect that is herein added to conventional analytical models is the ability to estimate changes in groundwater flow direction. Therefore, the first step of the proposed model is the creation of a methodology to get the major groundwater transport direction, starting from the contaminant source. This provides the central pathline of movement of the conta-

minant plume. Assuming that the groundwater will flow from the highest to the lowest groundwater level, groundwater head data points can be used in ArcGIS to define a groundwater head contour map. This is done by using geostatistical tools available in ArcGIS, to interpolate groundwater level measurements for the entire area of coverage. Then, the “Create Steepest Path tool” is used to define the preferred path of travel of a contaminant particle, starting from the contaminant source and flowing with the groundwater. The concept behind the process is very simple. As depicted in Figure 2, from a starting point, GIS seeks the lowest location and moves to that position, and then it repeats the process until a sink is located. The pathline is defined for an undefined amount of time. Now that groundwater flow direction is determined, advective transport equations are used to compute the maximum distance traveled by the contaminant due to advection, as explained next.

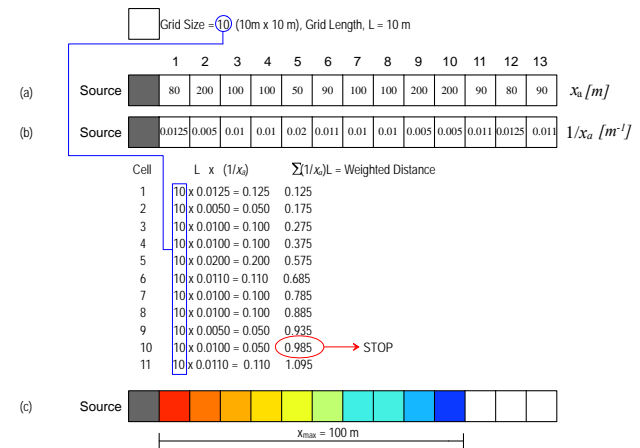


Figure 3. B-function and cost-weighted distance to find  $x_{max}$ ; (a) potential advective traversed distance based on properties of each cell; (b) inverse of potential distance; (c) final plume based on the weight of each grid.

### 2.3. Distance Traveled Due to Advection

A complication in computing the maximum distance traveled by the contaminant for a given time arises from the fact that flow velocity is not constant due to heterogeneous hydrogeological conditions. To solve this problem, a methodology that is based on the b-function proposed by Xiang and Stratton (1996) has been developed for use in the proposed technique. The methodology depicted by Figure 3, functions as described below: (1) For each cell, the advective distance is computed using the time of interest and its geohydrological characteristics. In the case of cell 1 of the example shown in Figure 3, this distance is 80 meters. This means that, if the whole area had the same characteristics as cell 1, the maximum advective distance traveled,  $x_a$ , would be 80 meters for the given time of interest; (2) The inverse of the values computed in step 1 are then defined for each cell. The inverse function indicates the fraction of the total time needed to travel a unit length (in this case 1 meter) in that specific cell. For example, in cell 1, if 80

meters is the maximum distance that would be traveled in a given time, to travel 1 meter in that cell would take a fraction of 0.0125 (1/80) or 1.25% of the given time of interest; (3) The fraction stored in each cell is multiplied by the cell size [meters], which gives the fraction of the total time spent traveling through that cell; and (4) These fractions are added up until the value reaches 1, which means that the fraction of time spent has reached 100% of the given time, and that is the farthest the contaminant would travel due to advection in this amount of time..

ArcGIS has a function called cost-weighted distance which is used to perform step 4 presented above and is explained later. In cases where the path leads to a cell located diagonally from the cell of origin, such as in Figure 2(c), ArcGIS uses the diagonal of the cell to compute the cumulative fraction of time. Also, because the function is performed using the center of the cells, for a single cell, GIS may use half of the diagonal plus half of the cell size as the distance traveled in that cell, as illustrated in Figure 2(c). The mathematical background supporting the methodology presented above is explained as follows. For the next set of equations, regions are herein considered to be areas with identical hydrogeological conditions. Then, after the basic calculations are performed, the regions are converted into a raster dataset for further processing.

The distance traveled for a given time by the center point of the plume due to advection for each different region,  $x_{a_j}$  is given by Equation (1):

$$x_{a_j} = v_{w_j} t_{e_j} \quad (1)$$

where  $x_{a_j}$  is the distance the center point of the plume would travel due to advection if the whole study area had the same properties as region  $j$ , as discussed before.

$$v_{w_j} = \frac{i_j \cdot k_{s_j}}{n_{e_j}} \quad (2)$$

where  $i_j$  is the hydraulic gradient or groundwater slope of region  $j$ ,  $k_{s_j}$  is the hydraulic conductivity of the soil in region  $j$  [L/T], and  $n_{e_j}$  is the effective porosity of region  $j$  soil.

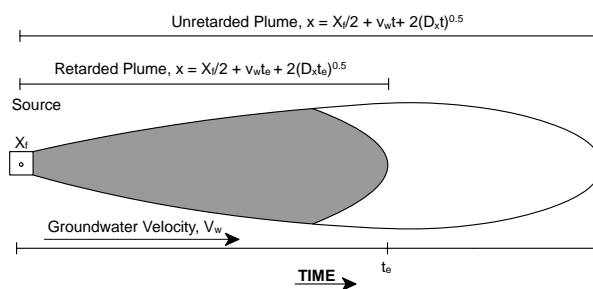
$$t_{e_j} = \frac{t}{R_{f_j}} \quad (3)$$

where  $t_e$  is the effective time [T]; and  $t$  is the time of interest input by user [T], and

$$R_{f_j} = 1 + \frac{\rho_{d_j} K_{d_j}}{n_j} \quad (4)$$

The effective time is used herein to address physico-chemical phenomena that constrain the movement of contaminant

particles in relation to the groundwater flow. Equation (4) is the retardation factor based on equilibrium equations of contaminant sorption to the surfaces of particles of the transport medium. The conceptualization of effective time is depicted in Figure 4.



**Figure 4.** Conceptualization of effective time for retarded plume.

After  $x_{a_j}$  is computed for each region in the study area, the area is converted to a grid with a given cell size (note that small cell sizes result in a higher resolution and consequently, smaller error, but greater processing time). As previously indicated, the final distance traveled due to advection is determined by adding the contribution of each cell, and stopping at the cell in which the summation reaches 1, as indicated in Equation (5):

$$\sum_{j=1}^m \frac{1}{x_{a_j}} S = 1 \quad (5)$$

where  $S$  is the grid cell size, and  $m$  is the number of cells traversed before the total contribution reaches 1.

#### 2.4. Distance Traveled in the Vadose Zone

In the cases where the contaminant is released above the groundwater and travels downward through the vadose zone, the amount of time in the vadose zone is also considered by adding its contribution as indicated below:

$$H_v = v_{w_v} \cdot t_{e_v} \quad (6)$$

where  $H_v$  is the distance that the contaminant would travel downward in a vadose zone with infinite thickness [L] for a given time, and other variables are as described previously. For a finite vadose zone, with thickness equal to  $h_v$ , only a fraction of the time is used by the contaminant in traveling through the intervening vadose zone,  $\delta_v$ . This fraction is given by Equation (7); note that transport equations for the vadose zone are not included herein, as the methodology is generic and any vadose zone model could be used:

$$\delta_v = \frac{1}{H_v} h_v \quad (7)$$

$$\delta_v = \frac{1}{v_{w_v} t_{e_v}} v_{w_v} t_v \quad (8)$$

$$\delta_v = \frac{t_v}{t_{e_v}} = \frac{t_v}{t/R_f} = \frac{R_f t_v}{t} \quad (9)$$

Therefore, the advection transport Equation (5) becomes Equation (10), when contaminant is not directly introduced into the groundwater and travel time in the vadose zone is considered:

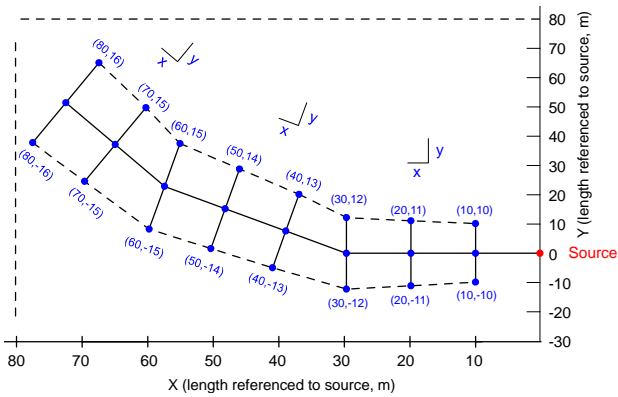
$$\sum_{j=1}^m \frac{1}{x_{a_j}} S = 1 - \delta_v = 1 - \frac{R_f t_v}{t} \quad (10)$$

$$S \left( \frac{R_f t_v}{St} + \sum_{j=1}^m \frac{1}{x_{a_j}} \right) = 1 \quad (11)$$

In a case in which the time,  $t$  is small, the transport may be limited to the vadose zone, and  $\delta_v$  will be equal to or greater than 1, indicating that the contaminant has not reached the groundwater, and that  $m$  (number of cells traveled) is equal to 0.

### 2.5. Distance Traveled Due to Dispersion in x, y, and z Directions

As indicated in Figure 5, due to the change in groundwater flow direction, it is not reasonable to use the coordinate system with the origin at the source to define dispersion, as done in conventional analytical models.



**Figure 5.** Conceptualization of axis rotation due to change in groundwater direction points (printed in blue), which are referenced to a new rotated coordinate system.

Another problem is that changes in hydrological conditions are not often considered in such analytical models. The effect of hydrogeological changes to dispersion is incorporated to the model as follows. The component of dispersion in the groundwater is computed for each cell by adding the contribution of

dispersion of one cell for which calculation is made:

$$x_d = \begin{cases} \sum_{j=1}^n 2(D_{x_j} t_{e_j})^{0.5} : n = m > 0 \\ 0 : n = m = 0 \end{cases} \quad (12)$$

The value of the coefficient of hydrodynamic dispersion,  $D$ , is computed as the average of the values for all cells preceding the cell being treated:

$$D_{x_j} = \frac{SD_{x_1} + SD_{x_2} + SD_{x_3} + \dots + SD_{x_j}}{nS} = \frac{1}{j} \sum_{q=1}^j D_{x_q} \quad (13)$$

$$t_{e_j} = t_{e_1} + t_{e_2} + t_{e_3} + \dots + t_{e_n} \\ = \frac{S}{v_{w_1} R_{f_1}} + \frac{S}{v_{w_2} R_{f_2}} + \frac{S}{v_{w_3} R_{f_3}} + \dots + \frac{S}{v_{w_j} R_{f_j}} \quad (14)$$

$$t_{e_j} = S \sum_{q=1}^j \frac{1}{v_{w_q} R_{f_q}} \quad (15)$$

$$x_d = \begin{cases} \sum_{j=1}^n 2 \left( \frac{S}{j} \sum_{q=1}^j D_{x_q} \cdot \sum_{q=1}^j \frac{1}{v_{w_q} R_{f_q}} \right)^{0.5} & (n = m > 0) \\ 0 & (n = m = 0) \end{cases} \quad (16)$$

where  $S$ , as defined before, is the grid cell size. Note that  $n$  is equal to  $m$ , which has been defined before as the farthest cell in the grid reached by the center of the plume due to advection in a given time. Similarly, the total dispersion in the  $y$ -, and  $z$ -directions, are given by Equations (17) and (18), respectively:

$$y_d = \begin{cases} \sum_{j=1}^n 2 \left( \frac{S}{j} \sum_{q=1}^j D_{y_q} \cdot \sum_{q=1}^j \frac{1}{v_{w_q} R_{f_q}} \right)^{0.5} & (n = m > 0) \\ 0 & (n = m = 0) \end{cases} \quad (17)$$

$$z_d = \begin{cases} \sum_{j=1}^n 2 \left( \frac{S}{j} \sum_{q=1}^j D_{z_q} \cdot \sum_{q=1}^j \frac{1}{v_{w_q} R_{f_q}} \right)^{0.5} & (n = m > 0) \\ 0 & (n = m = 0) \end{cases} \quad (18)$$

When  $m$  is equal to 0, it indicates that the given time of interest is not enough for the plume to travel through the vadose zone and reach the groundwater. After the contaminant plume is delineated, contaminant concentration is computed using one of the solutions of the ADE for points located at the outer border of the plume and along the path traveled by the center of the plume, which have known coordinates based on axes rotation incorporated into this methodology as described in section 2.6.

## 2.6. Spatial Interpolation of Contaminant Concentrations

The previous steps of the methodology model the farthest distance of travel of contaminant particles based on hydrogeological conditions and retardation factors for a given time of interest. Another important step is the characterization of the plume in terms of contaminant concentration. This can be achieved by using a solution of the ADE. Available literature provides an extensive list of solutions for different scenarios and boundary conditions such as radial flow and dispersion (Hoopes and Harleman, 1967); first-order decay reactions (Van Genuchten, 1985); multilayered medium (Gureghian and Jansen, 1985); 2D flow and 2D dispersion (Dillon, 1989); heterogeneous media (Yates, 1990); 3D semi-infinite porous media (Leij et al., 1991), homogeneous unsaturated medium (Zaidel and Russo, 1994), and desorption and decay (Fry and Istok, 1993). Any of these solutions can be used to compute contaminant concentrations within the plume. However, as discussed before, due to changes in groundwater flow direction, the coordinate values used in any of the solutions should be changed in time and space. Herein, the length of the path traveled by the contaminant is used as the extension of the plume in  $x$  direction and dispersion values are used as extensions of the plume in  $y$  and  $z$  directions.

As previously noted, contaminant concentrations are calculated for relevant points along the central path of the plume and at the border of the plume. The concentration values at other locations in the plume are computed through interpolation. Several techniques are available for use in interpolating data between scatter points (e.g. Spline, Kriging, etc.). A widely used interpolation method is the inverse distance weighted (IDW) interpolation. For a single interpolating point, IDW averages the concentration of adjacent scatter points, considering the distance to each of them. Therefore the weight of each scatter point reduces as the distance increases. The IDW interpolation method that is included in ArcGIS, is able to interpolate in both two and three dimensions.

## 3. Approach to GIS-CONTRAM Implementation

The GIS-based Contaminant Migration Model was implemented into GIS using the ModelBuilder tool of ArcGIS Desktop 9.1. Although the initial plan was to have the complete model built in ModelBuilder, some essential functions were not available, and some additional scripts were needed and developed using Visual Basic (VB) scripts. For this reason, this first version of this model is divided into 3 major integrated steps that include more than 200 ArcGIS geoprocesses. Plans are being made for the near future to combine these three steps into one, improving the usability of the model.

In the first step, three different feature layers are pre-processed and overlaid onto a single layer, and some model variables are calculated. The model has seven input parameters as described below.

**Soil Layer** – This is a polygon feature layer that includes the distribution of different types of soils in the region of concern. Although in the example presented herein, hydrological

soil groups were used to classify the soils, any other classification is accepted. The only mandatory field of this layer is a text-type field that is named *SoilType* and contains the classification codes.

**Monitoring Wells** – This is a point feature layer indicating the groundwater level at the monitoring wells. The only mandatory field of this layer is a numeric double-type field that should be named *Sea\_level* and contain the ground water elevation relative to the mean sea level [unit: m].

**Contaminant Source** – This is also a point feature layer that contains the location of potential contamination sources (e.g. landfills and surface impoundments). There are 4 obligatory fields in this layer: *failed*, a numerical short integer-type field that defines facilities as failed (1) or standing (0) (at this point, the model can only accept one failed facility at a time); *disposArea*, a numerical double-type field that contains the disposal area of the facility [unit: m<sup>2</sup>]; *LiquHead*, a numerical double-type field containing the contained liquid head (e.g. leachate head in a landfill or storage depth in a surface impoundment [unit: m]); *distToWt*, a numerical double-type field with the distance from the bottom of the facility to the groundwater table [unit: m]; *C0* denotes initial concentration of the chemical at the source [mg/L].

**Hydro\_info** – This input is a geodatabase table that can be developed using Microsoft Access. This table contains all the necessary hydrogeological information of the soil types contained in the soil layer input. The mandatory fields of this table are: *SoilType* – the soil types in this field should match the types used in the soil layer input; *Ks* – hydraulic conductivity for each soil type [unit: cm/s]; *Porosity* – porosity of the soil [ratio]; *EPorosity* – effective porosity of the soil [ratio]; *BulkDensity* – dry bulk density of the soil [g/mL]; *Kd* – sorption partition coefficient for the contaminant of interest [unit: mL/g]; *WaterContent* – water content of the soil [ratio]; (viii) *dx* – longitudinal (parallel to the flow) dispersivity [unit: m]; (ix) *dy* – transverse dispersivity ( $y$ -direction) [unit: m]; (x) *dz* – transverse dispersivity ( $z$ -direction).

**Raster Cell Size** – As discussed before, the model is based on discretization of the region into small cells. The smaller the cell size, the greater the precision of the model. Note that increased precision also increases the resolution time. Depending on the region size and computer processing capacity, ArcGIS may encounter problems to solve the model at very high resolutions. [unit: meters]

**Time After Release** – Through this input, the user defines the time the model should consider when delineating the contaminant plume. The unit of time should match the unit of the hydraulic conductivity value. Some problems have been identified when running the model using seconds due to the dimension of the number which exceeds the numerical capacity of GIS in some calculations. It is suggested that time be entered in months. The first step outputs a layer with the groundwater head triangulated irregular network (TIN) that is used in the second step to define the contaminant path line from the contaminant source, and a layer called hydrogeology that contains all the hydrogeological information needed to define the con-

taminant plume.

In the second step, GIS-CONTRAM uses the triangulated irregular network (TIN) developed in Step 1 for the groundwater and the "Create Steepest Path" tool of ArcGIS' 3D Analyst to create the central path of travel of groundwater from the contaminant source. The central path delineation defines the trajectory of the groundwater based on the overall pressure heads of the area. Use of the slopes of groundwater heads to produce the central head is analogous to tracking the preferred path of a ball released on the top of a hill. Depending on the resolution of the groundwater level map provided, the "create steepest path" tool will create unrealistic sharp turns due to linear interpolation between the points. This problem is minimized if more points are added to the monitoring well (groundwater level) layer. If monitoring wells are not available, the user may convert groundwater elevation contour lines into points and use this point as groundwater elevation points (monitoring wells). Because the Create Steepest Path tool generates a graphic feature that has no topology, and consequently cannot be integrated into the GIS model, a script is used to convert the graphic feature into a GIS-compatible polyline shapefile. The output of this step is a polyline shapefile that indicates the preferred path of the groundwater from the contamination source.

In the final step, GIS-CONTRAM uses the variables available in the hydrogeology layer created in Step 1 for the different hydrogeological regions, in combination with the preferred groundwater flow path obtained in Step 2, to delineate the contaminant plume. In summary, this step uses the process depicted in Figure 3 and discussed previously, to define the maximum distance traveled by the contaminant plume due to advection. Then, it uses the dispersion equations for the direction  $x$ ,  $y$  and  $z$ , presented in Equations (17), (18) and (19), respectively. At this point, with the center path line and the outer limits of the plume defined, contaminant concentrations for various points at different times of interest can be computed using an ADE solution, considering the rotating axes coordinate system.

#### 4. Application of the GIS-CONTRAM to Field Scenarios

##### 4.1. Approach to Model Validation

An acceptable validation process is to compare the results of a model to the results of a well-known and widely accepted model. In the case of this GIS-CONTRAM model, validation was done against the widely-used Visual MODFLOW models. Readers may wonder why verification has not yet been performed by comparing GIS-CONTRAM results to field data. Although this is planned on restricted basis, the use of other models (included in Visual MODFLOW) for the first step of quality assurance assessment of this model enables the consideration of the full ranges of data on significant parameters of the model in ways that circumvent the constraints of data unavailability at field sites. When data are available at some sites on significant parameters, they do not cover the desirable range of magnitudes for testing of new model over significant sce-

narios of contaminant transport.

Visual MODFLOW is the state-of-the-practice software for modeling groundwater flow and contaminant transport. It has been widely used and validated by U.S. and international agencies and private companies for use in modeling contaminant transport in the groundwater. Three components included in Visual MODFLOW (VM), were used herein: (i) MODFLOW (MF) – uses a finite-difference method to solve groundwater flow equations for porous media, outputting groundwater flow directions and velocities based on defined boundary conditions; (ii) MODPATH (MP) – uses groundwater properties defined by MODFLOW to identify the preferred path of a particle or set of particles located in the groundwater; and (iii) MT3DMS – compatible with MF, it computes the fate and transport of contaminants based on transport boundary conditions, soil and chemical properties, and groundwater environment defined by MF.

Combined MODFLOW (MF) and MT3DMS can solve flow and transport equations for a variety of scenarios, using a set of available flow boundary conditions (e.g. Constant Head, River, General-Head, Drain, Wall, Stream, Recharge and Evapotranspiration) and transport boundary conditions (e.g. Constant Concentration, Recharge Concentration, Evapotranspiration Concentration, and Point Source) for steady-state or transient flow conditions. However, VM does not include a solution for combined unsaturated and saturated flow conditions. One way of overcoming this limitation is to import recharge rates from unsaturated models into VM. As discussed before, the level of efforts and training needed to run Visual MODFLOW can sometimes inhibit its use, especially for initial stages of cost estimation and design of contaminant remediation technologies (Elmore, 2007). For such cases, analytical models and semi-analytical models, such as the GIS-CONTRAM, can provide a viable alternative to numerical models. The latter is especially of high utility when hydrogeological characteristics of the area of concern cannot be assumed to be homogeneous. It is important to note that GIS-CONTRAM uses a two-dimensional approach to define the central path of the plume. Also, it assumes that the groundwater flows in the same direction as in the central path for the whole width and depth of the plume. The assumption seems reasonable as the contaminant transport in  $y$  and  $z$  directions due to dispersion is usually small when compared to the transport in the  $x$  (central path) direction. Nevertheless, the user should pay attention to flow convergence and divergence situations, especially near model boundaries. An additional feature of GIS-CONTRAM is straightforward linkage with unsaturated zone transport models, which are used to estimate the time of travel in the intervening vadose zone. Therefore, the time of travel in groundwater is equal to time since release minus the time spent traveling in the unsaturated layer.

In addition, GIS-CONTRAM output allows easy computation of projected area and volume of the contaminant plume, using GIS tools. This information enables the rational estimation of the costs of implementing contaminant remediation technologies.

**Table 1.** Model Parameters Values for the Hydrologic Soil Groups

Hyd. Soil Group	Hyd. Cond., $K_s$ (cm/month)*	Effective Porosity, $n_e$ **	Porosity, $n$ **	Bulk Density, $\rho_s$ (g/cm <sup>3</sup> )**	Partition Coefficient, $K_{d,C6H6}$ (mg/g)***	$d_x$ (m)***	$d_y$ (m)	$d_z$ (m)	IMD****
A	789	0.29	0.41	1.55	0.13	0.034	0.014	0.014	0.31
B	500	0.27	0.41	1.55	0.38	0.056	0.0224	0.0224	0.18
C	224	0.3	0.51	1.28	0.63	0.06	0.024	0.024	0.14
D	45	0.25	0.48	1.40	0.88	0.128	0.064	0.064	0.09

\* NRCS (1997); \*\* Goss (1990); \*\*\* Christensen et al. (2001); \*\*\*\* Butler et al. (2004).

#### 4.2. Computer Hardware and Computing Requirements

According to Waterloo Hydrogeologic, Inc, the developer of Visual MODFLOW, the minimum requirement for operating the software is a Pentium II, 300 MHz (or equivalent), Windows 2000/XP, 64 MB of RAM (128 MB recommended), 100 MB disk space, and a DVD-ROM is required for installation. For this research, a Pentium D, 3.00 GHz, 2 GB of RAM and Windows XP SP2 was used. Running MODFLOW, MODPATH and MT3DMS for the scenarios analyzed herein, took less than a minute. However, setting up the model can be very time-consuming, depending on the level of hydrogeological complexity associated with the targeted contaminant transport. As discussed before, GIS-CONTRAM was developed using ArcGIS desktop processes. ESRI, the developer of ArcGIS, indicates that the minimum requirement to run GIS-CONTRAM is a Pentium 1.0 GHz, 512 MB of RAM (1 GB recommended), 1.2 GB of disk space, and Windows 2000/2003/XP. The same scenarios (3,000 m  $\times$  3,000 m) that took approximately 1 minute to run using Visual MODFLOW (cell resolution of 50 m  $\times$  50 m), took about 15 minutes to run using GIS-CONTRAM (cell resolution of 5 m  $\times$  5 m). If a resolution of 10  $\times$  10 m is used, GIS-CONTRAM will run in about 5 minutes. It is important to note that run time will be also dependent on the size of the region analyzed for both Visual MODFLOW (VM) and GIS-CONTRAM.

#### 4.3. Hypothetical Scenarios Analyzed

Two anisotropic synthetic scenarios having site areas of 9 km<sup>2</sup> (3,000  $\times$  3,000 m) each, were used for comparison of GIS-CONTRAM, Visual MODFLOW and an analytical solution of ADE. It is important to highlight that the comparison to Visual MODFLOW is for validation purposes only, as Visual MODFLOW is a more comprehensive tool that should be selected when high accuracy levels are required. Synthetic scenarios were used herein to compare the three different models because it is easier to assess the results when the initial conditions are controlled and well known. The first scenario is a very simple case where the soil is assumed to be homogeneous and highly permeable (see hydrological group A in Table 1), with a constant head boundary on the whole left border of the region of 475 m and a constant head boundary on the whole right border of 165 m. In the second scenario, area was divided into several random soil regions. These soil regions were classified according to the hydrological soil group classification. The parameters used for each soil classification is presented in Table 1. In terms of flow boundary conditions, assuming the left-bo-

ttom corner as the model origin ( $x = 0, y = 0$ ), constant head boundaries were set as: 475 m located at positions (0, 0) and (0, 3000), 25 m located at position (3000, 3000), 350 m located at position (3000, 0) and 600 m located at position (1350, 0). For both scenarios, the contaminant source is assumed to be a landfill with source dimensions of 200 W  $\times$  200 L  $\times$  0.3 H meters [0.3 meters is the maximum allowed leachate height within the landfill (EPA, 1988)], and center located at position (850, 1400). Landfill bottom is located 5 m above the groundwater table. The selected target contaminant is Benzene (C<sub>6</sub>H<sub>6</sub>) with initial concentration of 0.9 mg/L (concentration is based on values found on landfills compiled by Christensen et al. (2001). Benzene is a carcinogenic contaminant with low sorption levels, low degradation levels at anaerobic conditions commonly found in the groundwater, and its maximum contaminant level (MCL) in drinking water is 0.005 mg/L.

For these scenarios, an instantaneous release from a parallelepiped contaminant source is assumed. The ADE solution for this scenario has been developed by Domenico and Robbins (1985). It should be noted that, as discussed by Ahsanuzzaman et al. (2003), the equation presented by Domenico and Robbins (1985) has some misplaced brackets. Equation (19), which is a modification of the instantaneous cubic (finite) source developed by Hunt (1978), is correctly presented below.

$$C_i(x, y, z, t) = \frac{C_0}{8} \left[ \operatorname{erf} \left( \frac{x - v_w t + X_f/2}{2(D_x t)^{0.5}} \right) - \operatorname{erf} \left( \frac{x - v_w t - X_f/2}{2(D_x t)^{0.5}} \right) \right] \left[ \operatorname{erf} \left( \frac{y + Y_f/2}{2(D_y t)^{0.5}} \right) - \operatorname{erf} \left( \frac{y - Y_f/2}{2(D_y t)^{0.5}} \right) \right] \left[ \operatorname{erf} \left( \frac{z + Z_f/2}{2(D_z t)^{0.5}} \right) - \operatorname{erf} \left( \frac{z - Z_f/2}{2(D_z t)^{0.5}} \right) \right] \quad (19)$$

As discussed by Wexler (1992) and Fetter (1994), the initial conditions, boundary conditions and assumptions that apply to Equation (19) are provided as follows.

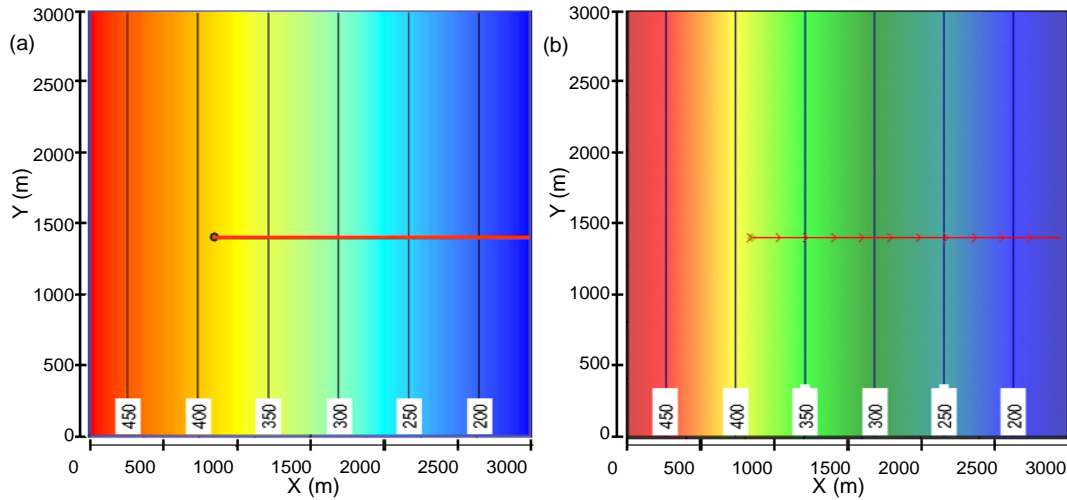
Boundary Conditions: concentration and concentration change are equal to zero at a location far from the source at any time:

$$C, \partial C / \partial x = 0 : x = \infty \quad (20)$$

$$C, \partial C / \partial y = 0 : y = \infty \quad (21)$$

$$C, \partial C / \partial z = 0 : z = \infty \quad (22)$$

Initial Condition: concentration is assumed to be zero at



**Figure 6.** Groundwater head contour lines and pathline from source for scenario 1: (a) GIS-CONTRAM and (b) Visual MODFLOW.

any point outside the finite source:

$$C = 0 : \left( \frac{X_f}{2} < x < \infty \right), \left( \frac{Y_f}{2} < y < \infty \right), \left( \frac{Z_f}{2} < z < \infty \right), t = 0 \quad (23)$$

Assumptions: aquifer has infinite width and height; conservative solute (no decay); flow with constant velocity in  $x$ -direction only; dispersion coefficients ( $D_x, D_y, D_z$ ) are constant.

Also, because vadose zone transport is less significant than plume transport in the GIS-CONTRAM methodology, limited imprecision in estimates of contaminant transport rates in the vadose does not influence the overall model results significantly. Herein, it is assumed that in the vadose zone, the contaminant front can easily flow downwards. In this case, the time the contaminant front takes to reach the groundwater,  $t_v$ , can be estimated using the infiltration model proposed by Green and Ampt (1911) indicated below:

$$t_v = \left( \frac{w_s - w}{k_s} \right) (h_v - (h - h_d)) \ln \left( 1 - \frac{h_v}{h - h_d} \right) \quad (24)$$

where  $k_s$  is the saturated hydraulic conductivity of the soil (L/T),  $w$  is the initial water content of the soil,  $w_s$  is the saturation moisture content of the soil,  $h_d$  is the capillary suction of the unsaturated soil,  $h_v$  is the vadose zone thickness, and  $h$  is the height of impounded liquid waste.

As the GIS-CONTRAM is based on analytical solutions of the ADE, for a scenario where soil is homogeneous and groundwater direction and velocities are constant, such as in Scenario 1, the outputs should be very similar for both models. Therefore, Scenario 1 was designed to validate all the processes used in GIS-CONTRAM. On the other hand, Scenario 2, which includes soil heterogeneity and changes in flow direc-

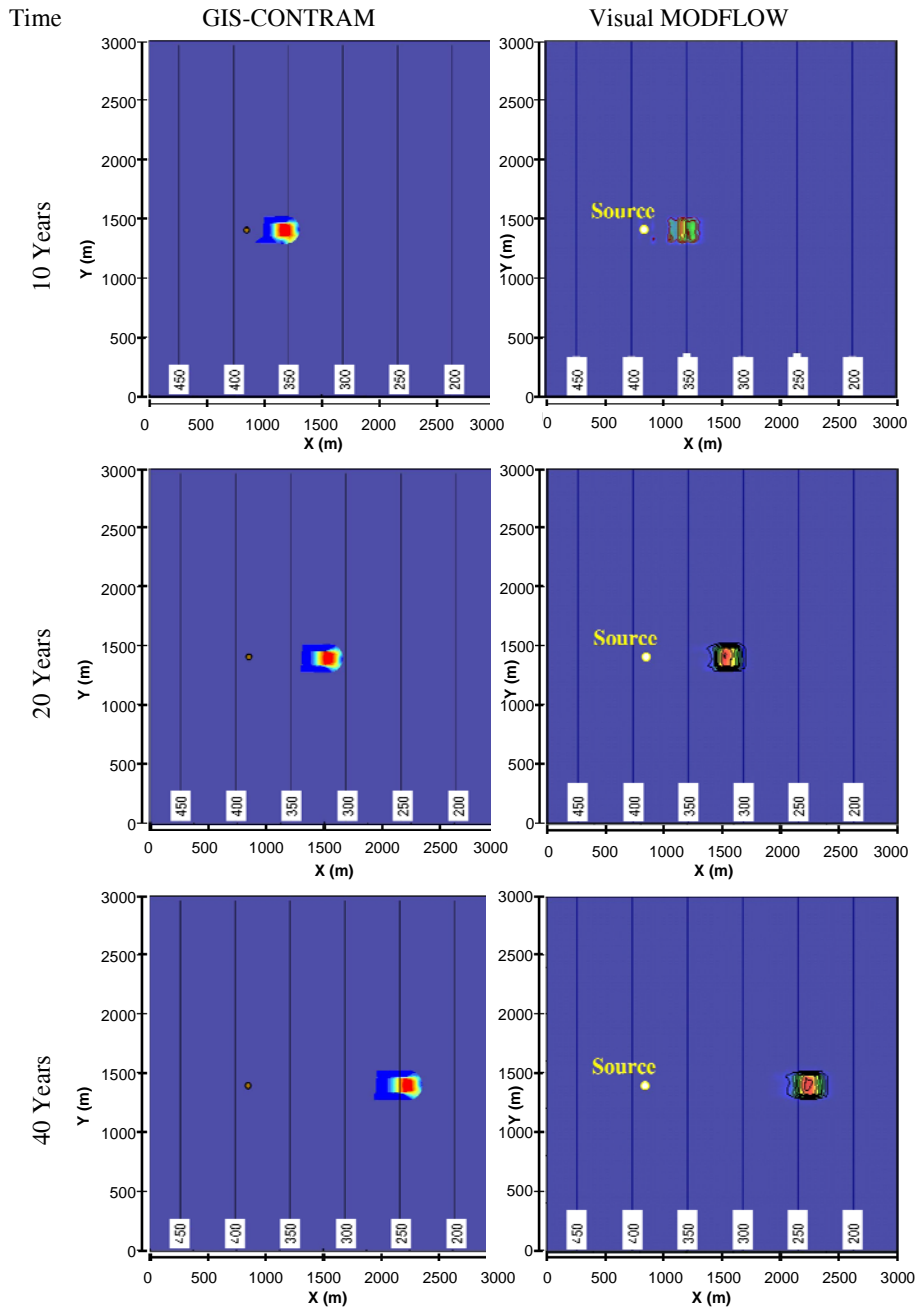
tion, was used to assess the behavior of GIS-CONTRAM under more complex conditions, through comparison with Visual MODFLOW. Furthermore, through Scenario 2 it was possible to assess if the GIS-CONTRAM's ability to address hydrogeological heterogeneity will produce better results than an analytical solution when they are compared to Visual MODFLOW.

## 5. Analyses of Results

Model comparison was performed through assessments of contaminant path line, plume geometry and location at 10, 20 and 40 years after release and through comparison of contaminant concentration at 15 observation wells also at 10, 20 and 40 years. As in the considered scenario, the contaminant is instantaneously released, and it is assumed that the plume moves as a plug flow. The observation wells were intentionally chosen such that they are located within the contaminant plume output by GIS-CONTRAM. Then, the geographic location and concentration of wells were exported to VM for comparison. In the analysis, regression lines for each time and the standard error of estimate were used.

Results indicate that there is a very good match for GIS-CONTRAM [Figure 6(a)] and Visual MODFLOW [Figure 6(b)] for both head and contaminant pathline for Scenario 1. In terms of plume location and geometry. Figure 7, depicting the contaminant plume at 10, 20 and 40 years, indicates that the GIS-CONTRAM output is similar (position and shape) to the one of Visual MODFLOW. It is also noted that VM's plume is moving a little faster than GIS-CONTRAM's, due to a small difference (0.024 m/month) in the groundwater flow velocity computed by GIS-CONTRAM (2.884 m/month) and VM (2.908 m/month). This small variation, over 40 years, causes VM's plume center to travel an additional approximate distance of 12 meters (due to error propagation), when compared to





**Figure 7.** Scenario 1 contaminant plume position and geometry at 10, 20 and 40 years after release for GIS-CONTRAM and Visual MODFLOW.

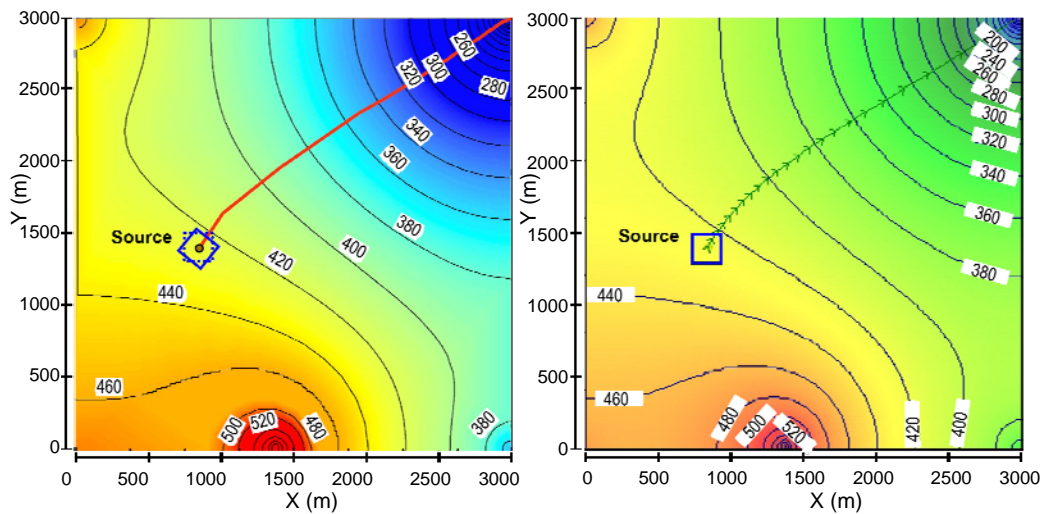
GIS-CONTRAM.

The outputs for Scenario 2 also indicate a reasonable match between GIS-CONTRAM and VM. It is possible to observe through the contaminant pathline for Scenario 2 depicted in Figure 8 that flow direction modeled by GIS-CONTRAM presents sharp changes in the flow direction, while VM presents a smoother pathline, which should be more consistent with reality. Nevertheless, pathline for the Scenario 2 modeled by GIS-CONTRAM is very similar to the one modeled by VM. In

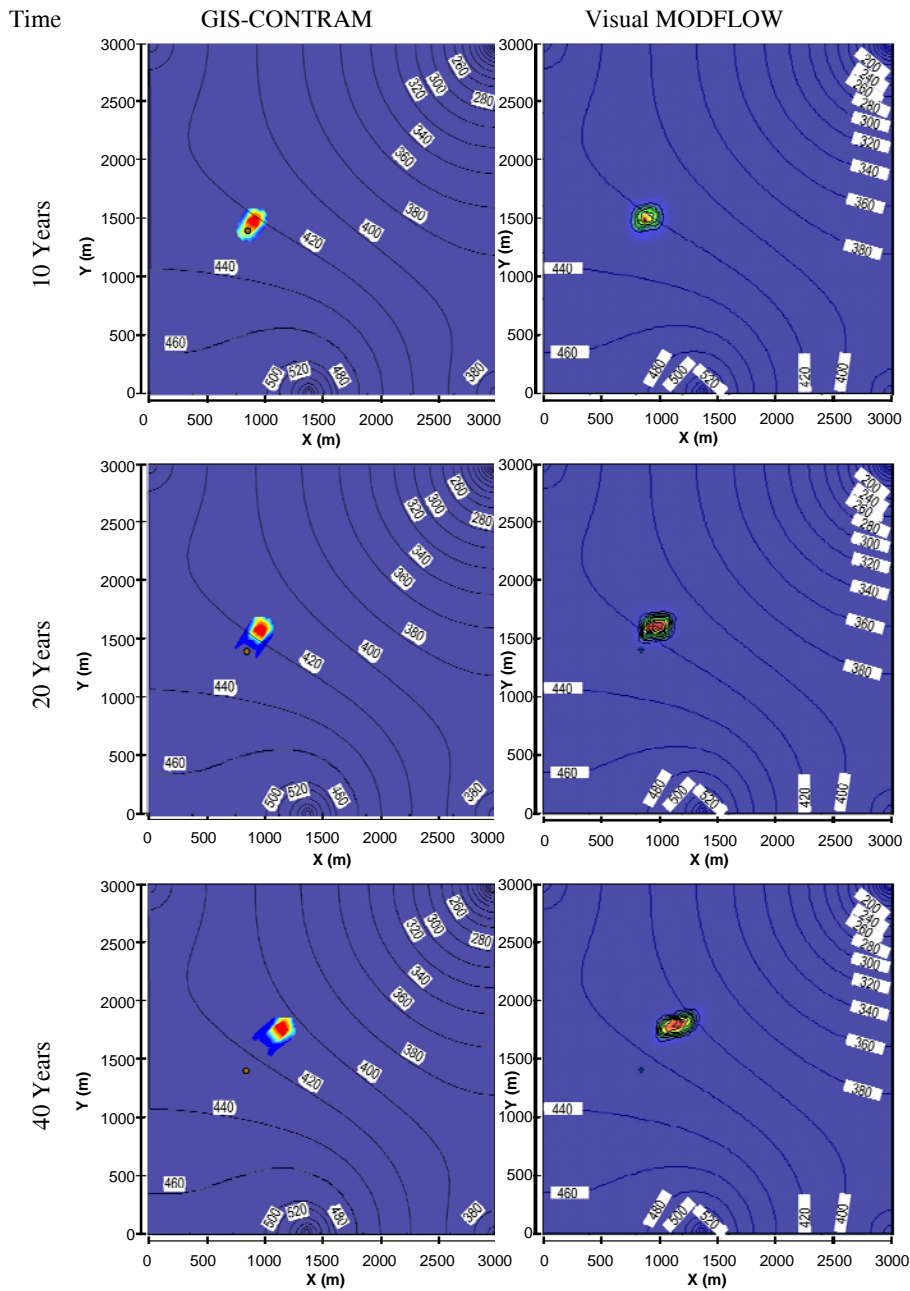
terms of geometry and location of the contaminant plume, it is possible to note from Figure 9 that, although the contaminant plume location is similar for both models, GIS-CONTRAM's plume outline is very smooth, while VM's plume shape is irregular. The major reason for this difference is the fact that GIS-CONTRAM semi-analytical approach assumes the y-dimension of the contaminant source to be perpendicular to the initial flow direction, while VM uses the orientation of the cells marked as source, independent of flow direction (see contaminant

**Table 2.** Benzene ( $C_0 = 0.9$  mg/L) Concentration for 15 Locations Downgradient from Contaminant Source Modeled by AS, GIS-CONTRAM and Visual MODFLOW

	Time Years	Concentration (mg/L)			Error			R <sup>2</sup>			
		Well	AS	GIS-CONTRAM	VM	AS-GIS	AS-VM	GIS-VM	AS-GIS	AS-VM	GIS-VM
SCENARIO 1	10	1	0.0002	0.0002	0.0043	16%	96%	95%	0.9999	0.9494	0.9467
		2	0.0072	0.0074	0.0074	3%	4%	1%			
		3	0.0213	0.0215	0.0241	1%	12%	11%			
		4	0.0247	0.0248	0.0241	0%	2%	3%			
		5	0.0259	0.0259	0.0317	0%	18%	18%			
	20	6	0.0001	0.0002	0.0015	15%	91%	86%	0.9849	0.9517	0.9556
		7	0.0061	0.0039	0.0084	57%	27%	54%			
		8	0.0127	0.0129	0.0226	1%	44%	43%			
		9	0.0166	0.0167	0.0226	1%	27%	26%			
		10	0.0182	0.0181	0.0311	1%	42%	42%			
	40	11	0.0001	0.0001	0.0021	15%	95%	-	0.9990	0.8784	0.8615
		12	0.0043	0.0046	0.0092	5%	53%	51%			
		13	0.0072	0.0075	0.0092	3%	22%	19%			
		14	0.0106	0.0108	0.0205	2%	48%	48%			
		15	0.0122	0.0122	0.0297	0%	59%	59%			
SCENARIO 2	10	1	0.0040	0.0220	0.0164	82%	76%	34%	0.7141	0.3304	0.6277
		2	0.0350	0.0268	0.0164	31%	114%	64%			
		3	0.0167	0.0280	0.0427	40%	61%	34%			
		4	0.0420	0.0444	0.0427	5%	2%	4%			
		5	0.0438	0.0449	0.0897	3%	51%	50%			
	20	6	0.0000	0.0000	0.0007	0%	0%	-	0.908106	0.6499	0.6263
		7	0.0019	0.0050	0.0167	61%	88%	70%			
		8	0.0111	0.0206	0.0167	46%	34%	23%			
		9	0.0219	0.0284	0.0167	23%	31%	70%			
		10	0.0307	0.0306	0.0288	1%	7%	6%			
	40	11	0.0000	0.0002	0.0084	-	-	-	0.811485	0.6398	0.7752
		12	0.0009	0.0045	0.0062	81%	86%	28%			
		13	0.0033	0.0107	0.0243	69%	87%	56%			
		14	0.0094	0.0181	0.0210	48%	55%	14%			
		15	0.0207	0.0212	0.0291	2%	29%	27%			



**Figure 8.** Groundwater head contour lines and pathline from source for scenario 2: (a) GIS-CONTRAM and (b) Visual MODFLOW.

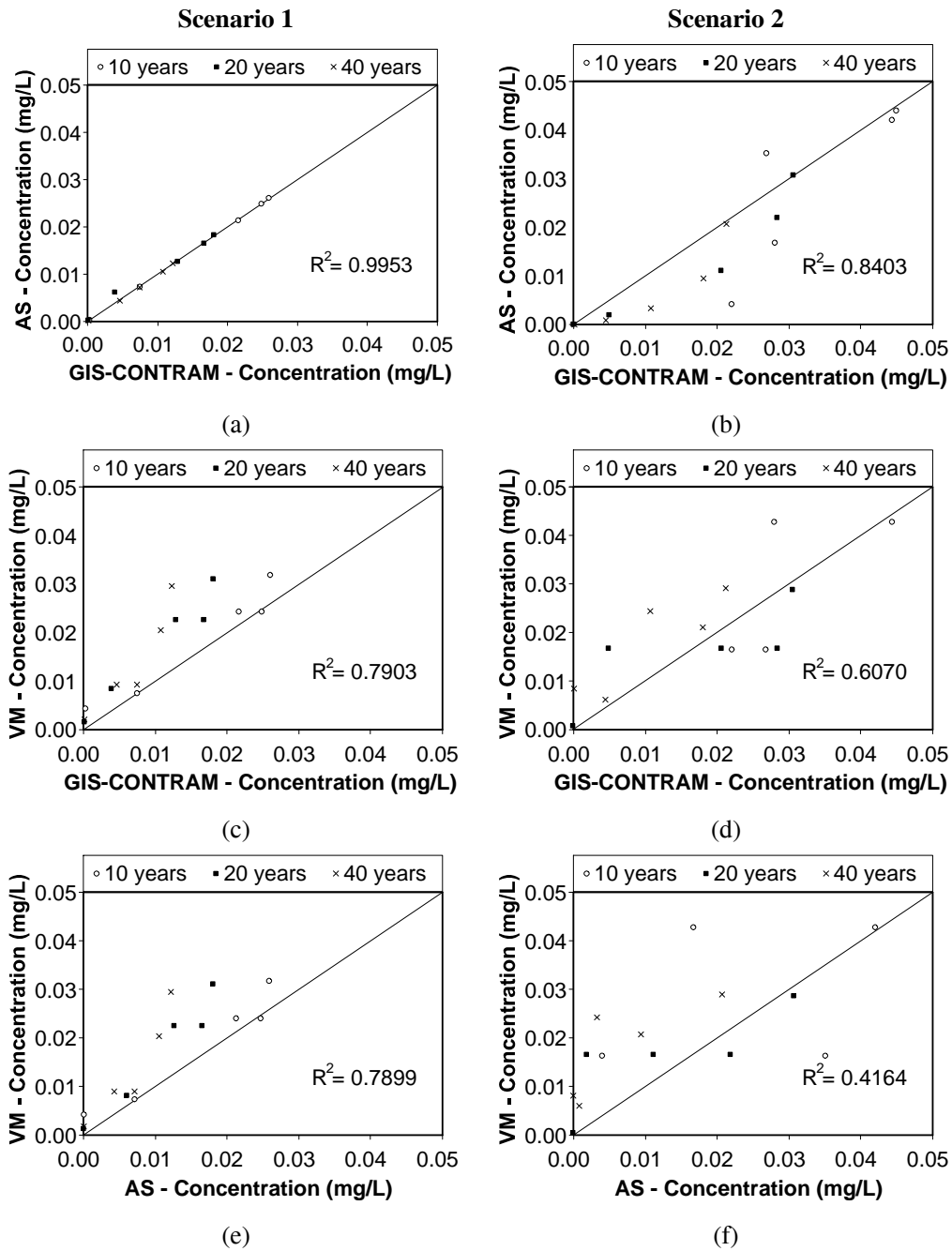


**Figure 9.** Scenario 2 contaminant plume position and geometry at 10, 20 and 40 years after release for GIS-CONTRAM and Visual MODFLOW.

source orientations for the two models in Figure 9).

In the next step, the concentrations at 15 locations were used to compare the three models in terms of contaminant concentrations downstream from the source for Scenarios 1 and 2. Five points were selected within the plume generated by ArcGIS for each time interval (10, 20, and 40 years). Then, the location and contaminant concentrations of these points were ex-

ported to Visual MODFLOW. The results are plotted in Figure 10 and tabulated as Table 2. As discussed before, GIS-CONTRAM semi-analytical approach is based on analytical solutions of ADE, but with the ability to incorporate changes in hydrogeological conditions. Therefore, Scenario 1 (homogeneous hydrogeological conditions) was mostly used to validate GIS-CONTRAM's processes. As indicated by Figure 10(a), the



**Figure 10.** Comparison of Analytical Solution (AS), GIS-CONTRAM, and Visual MOFLOW (VM) modeled benzene ( $C_0 = 0.9$  mg/L) concentrations at 15 locations downgradient from the source for three different points in time (10, 20 and 40 years after release).

concentrations modeled by analytical solution (AS) and GIS-CONTRAM have a nearly perfect fit for all three points in time ( $R^2_{10 \text{ years}} = 0.9999$ ;  $R^2_{20 \text{ years}} = 0.9999$ ;  $R^2_{40 \text{ years}} = 0.9992$ ). Also, the standard error of the estimated, which measures the overall distance between the values predicted by the two models, is very small ( $\sigma_{\text{est}, 10 \text{ years}} = 0.000157$ ;  $\sigma_{\text{est}, 20 \text{ years}} = 0.000070$ ;  $\sigma_{\text{est}, 40 \text{ years}} = 0.000101$ ). These results indicated that there are

no errors on the implementation of GIS-CONTRAM. Indeed, when compared to Visual MODFLOW (VM), GIS-CONTRAM [Figure 10(b)] and AS [Figure 10(e)] present the same correlation level and very similar standard error of the estimate for Scenario 1. Also from Figures 10(c) and 10(e), it is observed that although  $R^2$  is greater than 0.93 (good correlation) for all time intervals, the standard error of estimate indicate that the

difference between the concentration values modeled by AS and GIS-CONTRAM, and the ones modeled by VM tend to increase with time ( $\sigma_{\text{est}, 10 \text{ years}} = 0.0030$ ;  $\sigma_{\text{est}, 20 \text{ years}} = 0.0046$ ;  $\sigma_{\text{est}, 40 \text{ years}} = 0.0054$ ). Which can be explained by error propagation, as discussed before.

When hydrogeological variability is included, which is the case of Scenario 2, Figure 10(b) shows that the results for GIS-CONTRAM and AS do not match as well as they did for Scenario 1, which is understandable as AS does not address changes in groundwater direction and soil variability. Furthermore, Figures 10(d) and 10(f) show that GIS-CONTRAM achieves a better result than AS when compared to Visual MODFLOW,  $0.63 < R^2_{\text{GIS}} < 0.78$  and  $0.329 < R^2_{\text{AS}} < 0.65$ . This is a result of GIS-CONTRAM's ability to incorporate hydrogeological heterogeneity into the transport model. It is also important to note that for 10 and 20 years VM shows same concentration for nearby points (points within same cell have same concentration values), which is not true for GIS-CONTRAM and AS. This fact causes the points to fall in both sides of the perfect match line.

## 6. Conclusions and Recommendations

In this paper, a GIS-based contaminant transport model (GIS-CONTRAM) is introduced. Although, GIS-CONTRAM is based on analytical solutions of the advection dispersion equation (ADE), the methodology enables the incorporation of changes to hydrogeological conditions into the model. Because of this ability, the model is able to produce better estimates of contaminant fate and transport in groundwater than a straightforward analytical solution of the ADE for contaminant concentrations at various points and time. Its easy-to-use GIS-based interface allows some environmental scientists who may not be deeply familiar with computational methods to link contaminant transport and fate to other environmental assessment models without the need for more complex numerical solutions, and models like Visual MODFLOW that require extensive data formatting. This is especially true when the environmental assessment model is already built into a GIS platform.

The methodology has been fully implemented, and GIS-CONTRAM results have been compared to those Visual MODFLOW, which is the current state of the art groundwater modeling methodology, as well as results of an analytical solution of ADE. Also it was possible to visualize GIS-CONTRAM ability to incorporate hydrogeological changes and produce better results than analytical solution to ADE when compared to Visual MODFLOW. Extension of this work will focus on modeling contamination at real sites for verification of GIS-CONTRAM. A user guide (document) will also be developed to facilitate public use of this methodology.

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