Hydrologic Contaminant Transport Modeling: A Novel Analytical and Computational Approach

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Received February 13, 2002 Accepted April 5, 2002

ABSTRACT

We have developed a method for modeling contaminant transport in aquifers with rectangular boundaries utilizing an analytical solution to the porous medium flow equation and a finite difference solution to the advection-dispersion equation. Any number of wells may be placed within the aquifer, as well as any number of non-interacting contaminants. Constant head boundaries that simulate rivers may be included by means of a source term. With realistic parameters we are able to successfully model and predict contamination transport in an on-campus well site used for both undergraduate pedagogy and research.

I. BACKGROUND AND MOTIVATION

The University of Northern Iowa has a cluster of water monitoring wells which is near a river. A team of earth science students is estimating the effects of contamination within the aquifer spreading to the river. To assist them in their efforts we have developed a model which allows prediction of the spread of contaminants within the aquifer and into the river. The method presented here is chosen in favor of commercially developed packages such as MODFLOW because it is a wedding of computational and analytical work, it affords students the opportunity to explore the various facets of mathematical modeling firsthand, and it encourages faculty-faculty and student-student collaboration across departments. The purpose of this work is twofold: to outline the mathematical model we have developed and to also use that model to attempt a better understanding of a real system.

II. THEORY

There are a wide variety of approaches to modeling groundwater flow, both analytical [1,2] and numerical, involving discretization of space and using finite-element approaches [3,4]. Strictly speaking, we seek to describe contaminant flow in a confined aquifer with an impermeable rectangular boundary. However with the option of inserting a constant-head river within the aquifer the model at hand can be thought of as that of a semi-confined aquifer.

The approach described in this paper consists of two steps. First the behavior of the physical flow of water is modeled analytically with the porous medium flow equation. Secondly the water velocity field obtained from the first step is used in a finite-difference approach to solving the advection-dispersion equation.

a. Describing The Flow of Water

To model the flow of water in the aquifer, we are interested in solving the porous medium flow equation for a homogeneous, isotropic matrix:

$$K\nabla^2 h(x,y,t) + \sum_{i=1}^{N} q_i \delta(\vec{r} - \vec{r}_{i0}) + Q\delta(y - y_r) = S_s \frac{\partial h(x,y,t)}{\partial t}. \tag{1}$$

Here K is the hydraulic conductivity of the soil, S_s is its specific storage and h(x,y,t) is the potentiometric head at a point (x,y) and time t. There may be N wells; the i^{th} well is placed at a position $\vec{r}_{i0}=(x_{i0},y_{i0})$ and has volumetric pumping rate q_i, so $q_i>0$ for an injection well and $q_i<0$ for a pumping well. . δ is the Dirac delta function and is used in this case to describe a flow *density* which is modeled as being zero everywhere but is singular at the location of the wells or along the river line. Although the well volumetric pumping densities are horizontally singular they may be thought of as having unit extent in the vertical direction, so if their vertical extent is not of unit length then the q_i must be divided by the (constant) saturated pumping length of each well. There can be a river located at $y=y_r$ which is just a line injection or pumping source with areal pumping rate Q.

The system is subject to the initial condition h(x, y, t=0) = h_0(x, y) and the no-flow boundary conditions at the walls of the aquifer:

$$\left.\frac{\partial h(x,y,t)}{\partial x}\right|_{y=0} = \left.\frac{\partial h(x,y,t)}{\partial x}\right|_{y=B} = \left.\frac{\partial h(x,y,t)}{\partial y}\right|_{x=0} = \left.\frac{\partial h(x,y,t)}{\partial y}\right|_{x=A} = 0. \tag{2}$$

A schematic representation of the problem statement may be found in Figure 1. Equations (2) require the solution to be of the form

$$h = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} a_{jk}(t) \cos\left(\frac{j\pi x}{A}\right) \cos\left(\frac{k\pi y}{B}\right). \tag{3}$$

We can rewrite equation (1) as

$$K\left[\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2}\right] + \sum_{i=1}^{N} q_i \delta(\vec{r} - \vec{r}_{i0}) + Q\delta(y - y_r) = S_s \frac{\partial h(x,y,t)}{\partial t}, \tag{4}$$

Substitute equation (3) into (4), and multiply each term by cos($l\pi$x/A)cos($m\pi$y/B). Applying the orthonormality relationships for integrations over products of sine and cosine [5] (and see the Appendix) produces differential equations for the time-dependent expansion coefficients a_{jk}:

$$\frac{da_{00}(t)}{dt} = \frac{\left(\sum_{i=1}^{N} q_i\right)}{S_s} \tag{5a}$$

and

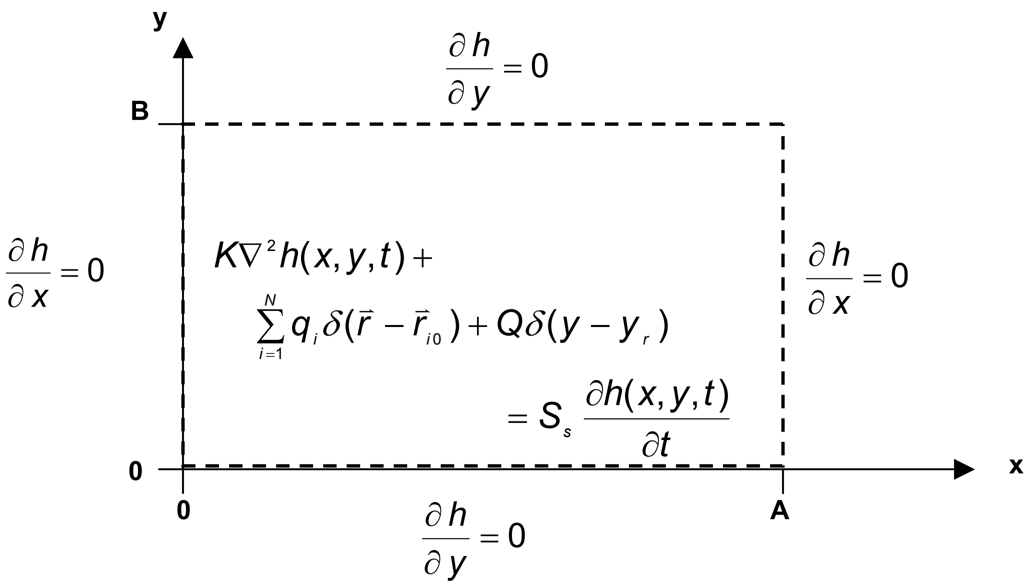

Figure 1. Schematic representation of the initial/boundary-value problem in modeling ground-water flow.

$$\frac{da_{0n}(t)}{dt} = \frac{-K}{S_s}\left(\frac{n^2\pi^2}{B^2}\right)a_{0n} + \frac{2}{ABS_s}\sum_{i=1}^{N} q_i \cos\left(\frac{n\pi y_{i0}}{B}\right) \quad (n \geq 1) \tag{5b}$$

$$\frac{da_{m0}(t)}{dt} = \frac{-K}{S_s}\left(\frac{m^2\pi^2}{A^2}\right)a_{m0} + \frac{2}{ABS_s}\sum_{i=1}^{N} q_i \cos\left(\frac{m\pi x_{i0}}{A}\right) \quad (m \geq 1) \tag{5c}$$

$$\frac{da_{mn}(t)}{dt} = \frac{-K}{S_s}\left(\frac{m^2\pi^2}{A^2} + \frac{n^2\pi^2}{B^2}\right)a_{mn} + \frac{4}{ABS_s}\sum_{i=1}^{N} q_i \cos\left(\frac{m\pi x_{i0}}{A}\right)\cos\left(\frac{n\pi y_{i0}}{B}\right) \quad (m,n \geq 1) \tag{5d}$$

Equations (5a) — (5d) can be solved to yield an expression for the coefficients themselves:

$$a_{00}(t) = a_{00}(0) + \frac{\left(\sum_{i=1}^{N} q_i\right)t}{S_s} \tag{6a}$$

$$a_{0n}(t) = a_{0n}(0)e^{\frac{-K}{S_s}\left(\frac{n^2\pi^2}{B^2}\right)t} + \frac{2\sum_{i=1}^{N} q_i \cos\left(\frac{n\pi\, y_{i0}}{B}\right)}{KAB\left(\frac{n^2\pi^2}{B^2}\right)}\left(1 - e^{\frac{-K}{S_s}\left(\frac{n^2\pi^2}{B^2}\right)t}\right) \quad (n \geq 1) \tag{6b}$$

$$a_{m0}(t) = a_{m0}(0)e^{\frac{-K}{S_s}\left(\frac{m^2\pi^2}{A^2}\right)t} + \frac{2\sum_{i=1}^{N} q_i \cos\left(\frac{m\pi x_{i0}}{A}\right)}{KAB\left(\frac{m^2\pi^2}{A^2}\right)}\left(1 - e^{\frac{-K}{S_s}\left(\frac{m^2\pi^2}{A^2}\right)t}\right) \quad (m \geq 1) \tag{6c}$$

$$a_{mn}(t) = a_{mn}(0)e^{-\frac{K}{S_s}\left(\frac{m^2\pi^2}{A^2}+\frac{n^2\pi^2}{B^2}\right)t} + \frac{4\sum_{i=1}^{N} q_i \cos\left(\frac{m\pi x_{i0}}{A}\right)\cos\left(\frac{n\pi y_{i0}}{B}\right)}{KAB\left(\frac{m^2\pi^2}{A^2}+\frac{n^2\pi^2}{B^2}\right)}\left(1 - e^{-\frac{K}{S_s}\left(\frac{m^2\pi^2}{A^2}+\frac{n^2\pi^2}{B^2}\right)t}\right). \quad (m,n \geq 1) \tag{6d}$$

Expressions for the initial expansion coefficients are obtained using equation (3) and the orthonormality relationships (see the Appendix):

$$a_{00}(0) = \frac{1}{AB}\int_0^A\int_0^B h_0(x,y)\,dy\,dx \tag{7a}$$

$$a_{0n}(0) = \frac{2}{AB}\int_0^A\int_0^B h_0(x,y)\cos\left(\frac{n\pi y}{B}\right)dy\,dx \quad (n \geq 1) \tag{7b}$$

$$a_{m0}(0) = \frac{2}{AB}\int_0^A\int_0^B h_0(x,y)\cos\left(\frac{m\pi x}{A}\right)dy\,dx \quad (m \geq 1) \tag{7c}$$

$$a_{mn}(0) = \frac{4}{AB}\int_0^A\int_0^B h_0(x,y)\cos\left(\frac{m\pi x}{A}\right)\cos\left(\frac{n\pi y}{B}\right)dy\,dx \quad (m,n \geq 1) \tag{7d}$$

In practice, equations (6a) — (6d) and (7a) — (7d) are numerically evaluated. The potentiometric head is then expressed as the sum in equation (3) which is truncated so that it contains n_x horizontal terms over the aquifer length and n_y vertical terms over the aquifer width; a constant-head boundary at the river is modeled by adjusting the head at $y = y_r$ to have a certain fixed value stepwise throughout the computer simulation. Table 1 shows the parameters important in modeling groundwater flow.

Parameter	Symbol	Value
Length of aquifer [6]	A	3 m
Width of aquifer [6]	B	5 m
Hydraulic Conductivity [6]	K	5×10^{-7} m/sec
Specific Storage [6]	S_s	4.9×10^{-3} m^{-1}
Number of terms in width (horizontal) sum	n_x	50
Number of terms in depth (vertical) sum	n_y	50

Table 1. Parameters important in modeling the groundwater flow.

b. Representing contaminant transport

The goal of the contaminant transport modeling in this work is to track the concentration of M non-interacting contaminant components. The governing equation for the behavior of the concentration $C_i(x,y,t)$ component (i) added to the aquifer is the advection-dispersion equation for an isotropic, homogeneous matrix,

$$D_i \nabla^2 C_i(x,y,t) + \vec{v} \bullet \vec{\nabla} C_i(x,y,t) = \frac{\partial C_i(x,y,t)}{\partial t}. \quad (i = 1, M) \tag{8}$$

Here D_i is the hydrodynamic dispersivity of contaminant component (i) and v is the average linear velocity of the water which we obtain from the potentiometric head:

$$\vec{v}(x,y,t) = -\frac{K}{\phi}\vec{\nabla} h(x,y,t) = -\frac{K}{\phi}\vec{\nabla}\left\{\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} a_{lk}(t)\cos\left(\frac{j\pi x}{A}\right)\cos\left(\frac{k\pi y}{B}\right)\right\}. \tag{9}$$

Here ϕ is the soil porosity and must be taken into account since not all the space is available for supporting water flow.

It is desirable to solve equation (8) analytically, but its complexity usually prevents such an effort. Therefore we use a simple finite difference approach. The aquifer is partitioned into a grid with N_x points in the horizontal direction and N_y points in the vertical direction, as shown in Figure 2. Then approximating the derivatives in equation (8) using finite differences we arrive at a discretized form of the advection-dispersion equation:

$$D_i\left(\frac{C_{i+1,j,k} - 2C_{i,j,k} + C_{i-1,j,k}}{(\Delta x)^2} + \frac{C_{i,j+1,k} - 2C_{i,j,k} + C_{i,j-1,k}}{(\Delta y)^2}\right) + v_x\left(\frac{C_{i+1,j,k} - C_{i-1,j,k}}{2\Delta x}\right) + v_y\left(\frac{C_{i,j+1,k} - C_{i,j-1,k}}{2\Delta y}\right) = \frac{C_{i,j,k+1} - C_{i,j,k}}{\Delta t}. \tag{10}$$

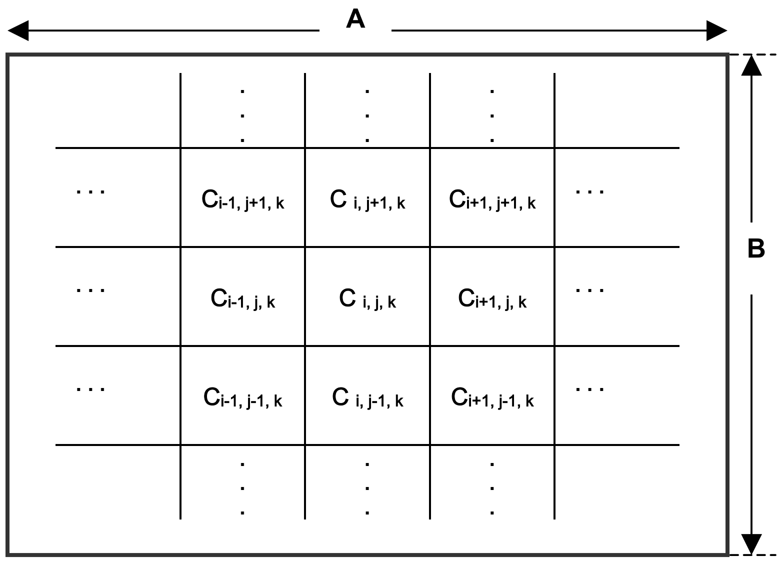

Figure 2. Diagrammatic representation of the finite difference grid used in modeling containment transport.

Equation (10) shows that $Ci(x_i,y_j,t_{k+1})$ is just equal to $Ci(x_i,y_j,t_k)$ plus an update which depends on the local environment of $Ci(x_i,y_j,t_k)$ with the average water velocity calculated as prescribed in equation (9). Therefore we begin with initial concentrations of contaminants C_{0i} for i = 1, M and advance equation (10) incrementally through time. Table 2 contains parameters relevant to the modeling of the transport of contaminants.

III. RESULTS AND DISCUSSION

We conducted a 6000 second (33.33 hour) simulation for chloride ion contamination with the aquifer parameters from Tables 1 and 2, with an initial head of 100 m (a guess) and a river with constant head of 5 m placed at y_r = 3 m. There is an injection well located at (1.5 m, 0.5 m), and the contaminant is initially placed at (1.5 m, 1 m). Final and early potentiometric head surfaces and contour plots are shown in Figure 3, and the corresponding series of contaminant concentration surfaces and contour plots are shown in Figure 4.

With the given hydraulic conductivity and head conditions, we found that diffusion was the dominant contaminant transport mechanism early in the simulation as the center of the contaminant plume remains fixed. Such behavior is due mainly to the fact that the aquifer we are modeling is fairly

Parameter	Symbol	Value
Soil Porosity [6]	ϕ	0.27
Initial concentration of Cl^- [6]	C_{10}	270 kg/m^3
Hydrodynamic dispersivity of Cl^- [6]	D_1	2.04×10^{-5} m^2/sec
Number of grid points in the horizontal direction	N_x	50
Number of grid points in the vertical direction	N_y	50

Table 2. Parameters important in modeling contaminant transport.

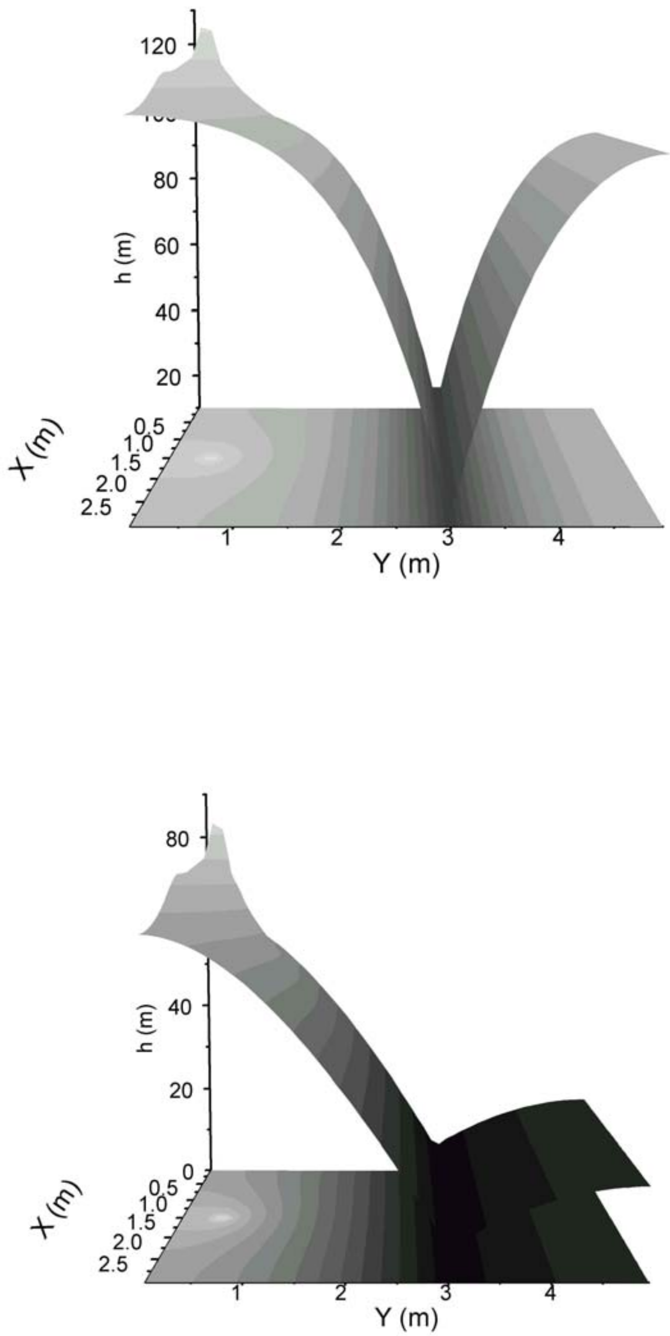

Figure 3. Potentiometric head surface and contour plots for the 2000 hour simulation shown at t = 1.67 hours (top) and 33.33 hours (bottom). The well and river are easily visible both on the surface plot and the contour plot on top and the grayscale ranges from 0 m (black) to maximum (white) as shown on the head axis of each plot. As is true for Figure 4, note that the aquifer is rectangular so the geometry is slightly distorted. The net effect of the river and the well are clearly evidenced by considerable drawdown.

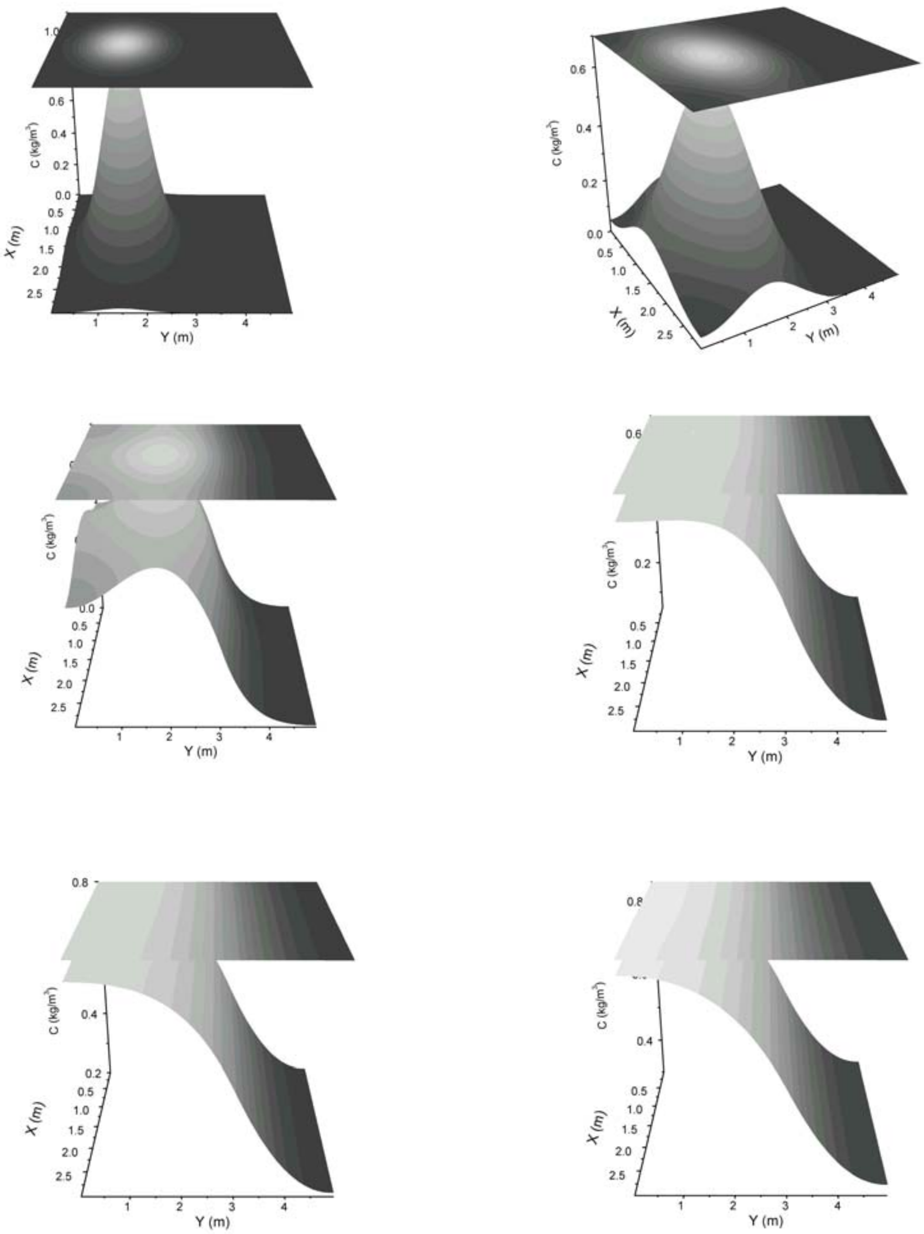

Figure 4. Contaminant profiles for the 33.33 hour simulation as shown at t = 1.67 hours, 3.333 hours, 8.33 hours, 16.67 hours, 25 hours and 33.33 hours, from upper left to lower right. The t = 3.33 hour plot is oriented slightly differently in order to show dimpling of the surface. The grayscales vary slightly from concentrations of 0 kg/m^3 (black) to maximum (white) as evidenced by the concentration-axis scales. The plots are presented this way so we can obtain optimal shade ranges for individual plots and to get a feeling for when and to what degree the contaminants are entering the river.

Figure 5. Contaminant plumes and contour maps at t = 1.67 hours (left) and t = 8.33 hours (right) in the same general format as previous figures. Compare to the contaminant plumes at the same times in Figure 4. Note the presence of advection here, where the center of the contaminant plume travels in the direction of the average water velocity.

small and diffusive transport is much more prevalent than that of advection. The plume continues to evolve in shape and the contaminant begins to reach the river after about 3 or 4 hours. Advection helps shape the contaminant plume as the river is reached and the plume ultimately takes on a shape cosmetically similar to that of the calculated water table, as would be expected in this scenario. Some contaminant does exist across the river but that part of our model does not reasonably represent the actual aquifer. As expected the pumping rate Q of the river decreases with time due to drawdown.

We also wanted to show the advective nature of contaminant transport as well, so we conducted a simulation with higher water speeds. We repeated the previous simulation using a hydraulic conductivity $k=5 \times 10^{-5}$ m/sec, unit porosity and an initial potentiometric head of 1000 m. We realize that the initial potentiometric head is artificially high in this case and we emphasize that this simulation is for the purpose of obtaining advection in our very small aquifer, as shown in Figure 5.

Early on, diffusion plays an important role in contaminant transport but the plume moves downstream towards the river as time progresses. Here the contaminant began reaching the river slightly prior to three hours, spread along the river faster and had higher concentrations along the river, all as expected. Ultimately the contaminant profile matches that of the calculated water table.

IV. CONCLUSIONS AND RECOMMENDATIONS

We have developed a model which is a wedding of computational and analytical approaches that actively involves undergraduate students in modeling multi-component, non-interacting contaminant transport in confined aquifers including any number of injection or pumping wells. Furthermore the model may incorporate constant head boundary conditions with the appropriate arrangements of rivers and/or wells whose potentiometric head are adjusted within the computer algorithm.

With realistic aquifer parameters used, it takes 3 to 4 hours for a chloride contaminant spot to reach the river when placed 2 m away from it initially. We emphasize however that the initial potentiometric head was only a guess and the transport time may vary according to actual conditions. The aquifer at the University of Northern Iowa is very small so advection does not seem to play an important role in contaminant transport. The pumping well seems to have little effect but could certainly matter more other situations (loner time, higher conductivity, etc.). With the model unrealistically exaggerated so as to give high water speeds we notice advection as well, and the contaminant behaves, as discussed earlier, in a way consistent with what is expected. In both scenarios the contaminant profile generally matches that of the water table after about 16 or 17 hours and no major is noticed at later times. It may be desirable to plot the contaminant concentration along the river and follow it with time; the model is applicable to a vast number of different situations so further student use for modeling specific systems is warranted and highly desirable.

APPENDIX

Integrations or sums over products of sines and cosines can be simplified by using the orthonormality relations for these functions [5]. In particular,

$$\int_0^A \int_0^B \cos\left(\frac{j\pi x}{A}\right)\cos\left(\frac{k\pi y}{B}\right)\cos\left(\frac{l\pi x}{A}\right)\cos\left(\frac{m\pi y}{B}\right)dx\,dy = \frac{AB}{4}\delta_{jl}\,\delta_{km}$$

and

$$\int_0^L \cos\left(\frac{j\pi u}{L}\right)\cos\left(\frac{l\pi u}{L}\right)du = \frac{L}{2}\delta_{jl}$$

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