

SOLVING THE CONTAMINANT TRANSPORT PROBLEM OVER A RANDOM CONDUCTIVITY FIELD

Michelle Hine
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ABSTRACT

In this paper, I explore the solution of the contaminant transport problem over a random conductivity field. First, I generate a random, correlated conductivity field by convolving independent, uniformly distributed random variables with the identity function. I use finite differences to discretize the diffusion equation to solve for the steady-state pressure gradient using Backward Euler. This allows calculation of the Darcy flux and hence the pore velocity over the random conductivity field. Finally, I solve the two dimensional advection-dispersion equation using an Adams-Bashforth, Adams-Moulton predictor corrector method to step forward in time. The generation of the random conductivity field and pressure gradient seem both accurate and efficient, and the finite difference method of solving the contaminant transport problem seems to be providing qualitatively correct solutions, but it is not volume conservative.

1. INTRODUCTION

Water. So necessary for life, yet so often overlooked. Here in the United States, one needs only to turn on the tap to access this cheap, abundant resource. However, even in developed countries, access to clean water can be a problem. The water that is not often considered—the water flowing unnoticed beneath one’s feet—can be just as hazardous to health as polluted drinking water. In 2005, 23% of the United States national total fresh-water usage came from groundwater, rather than surface water [8]. Many contaminants are water soluble, and hence, percolate through the unsaturated zone down to the water table. To maintain a healthy water supply, it is exceedingly important to understand the spread of contaminants through groundwater.

One of the most infamous hazardous waste incidents in the United States occurred when Hooker Chemical buried waste near what would later become the residential area of Love Canal, New York. By the 1970s, waste containment measures had failed to the extent that through groundwater transport, hazardous chemicals were leaking into basements and oozing onto playgrounds [5]. Studies from the New York State Department of Health show that former residents of Love Canal have elevated bladder cancer rates, elevated levels of certain contaminants in their bodies, a heightened rate of birth defects, and an increased risk of low weight and pre-term births [5]. While much of the Love Canal tragedy was due to human error, Love Canal highlights both the necessity of understanding the spread of contaminants through groundwater as well as understanding remediation measures.

Key words and phrases. groundwater hydrology, groundwater remediation, contaminant transport, advection-dispersion, stochastic modeling, risk-assessment model.

Given that a contaminant spill has occurred, it is vital to mitigate the effects of that spill. Many remediation techniques exist, including isolating the contaminants by creating a physical barrier; solidification by adding chemicals that bond to the contaminants and reduce mobility; and even bioleaching, where in-situ bacteria reduce sulfur compounds [4]. Each technique comes with a price, and depending of the type of spill and parameters of the location, one technique may be more favorable than others. This paper explores a first step building upon the work of Bolster, et al., to create a probabilistic risk assessment model of groundwater remediation failure [3]. The end goal is to create a simplified, spatially averaged model that accurately captures the failure of groundwater remediation measures. That is, given that certain remediation techniques are in place, the model will capture the likelihood that the concentration of a given contaminant will surpass its critical level at a specified location.

The research done for this paper models the flow of a contaminant through a saturated porous medium, as described by Darcy’s Law and the Advection-Dispersion equation. Due to natural variation, the pore structure of a medium varies at every point. This high degree of uncertainty leads many hydrologists to model the pore structure numerically, using random fields for the hydraulic conductivity and the hydraulic head (i.e. pressure field) [9].

2. A BRIEF INTRODUCTION TO GROUNDWATER HYDROLOGY

2.1. Preliminaries. Part of hydrology is modeling fluid flowing through the water table. For this paper, I study the flow of a contaminant through a saturated porous medium, assuming the both the fluid and contaminant are incompressible and that the contaminant does not react with the fluid. Hence, I can describe the flow of the contaminant with the advection-dispersion equation. For the remainder of this paper, I assume two-dimensional flow.

2.1.1. Diffusion and Dispersion. Diffusion is a thermodynamic process involving the mixing of particles, occurring on a microscopic scale. In diffusion, particles move from areas of higher concentration to areas of lower concentration. On the other hand, dispersion is a physical, mechanical process that also causes mixing of particles, but occurring on a continuum scale [1]. Both of these processes are fundamentally involved with the contaminant transport problem.

2.1.2. Uncertainty of Pore Structure. In groundwater hydrology, fluid flows through a saturated porous medium, but the pore structure of the medium is unknown. One of the ways hydrologists represent the uncertainty of a medium is by using the porosity: n is a number between 0 and 1, described by equation (1), where V_V is the void volume through which water and other substances can flow, and V_T is the total volume of the material.

$$(1) \quad n = \frac{V_V}{V_T}$$

Lower porosity indicates that less fluid can travel through the medium at any given time. The porosities of a couple common materials are listed in Appendix A. To test the code, I used a porosity of 0.25, which is commensurate with either gravel or a gravel and sand mixture.

Hydraulic conductivity K is a parameter that measures the ease with which fluid flows through a medium. While porosity and hydraulic conductivity are loosely connected, there is no strict correlation between the two [7]. Porosity yields only a view of fractional volume, while hydraulic conductivity also takes into account the geometry of the system. A medium with low porosity is likely to also have low conductivity, but clay is a media with

high porosity that also has low conductivity [7]. Hence, one must take both the porosity and the conductivity of the material into consideration.

I model the uncertainty of the pore structure using an underlying random vector field to generate a random, correlated conductivity field, as described in the Numerical Methods section. I then solve the diffusion equation numerically to obtain the pressure gradient, and use the pressure gradient to compute the hydraulic flux, and then calculate the pore velocity. Finally, the pore velocity is used to solve the contaminant transport problem using the advection-dispersion equation.

2.2. Governing Equations.

2.2.1. *Diffusion Equation.* The pressure gradient is determined by the diffusion equation acting on the hydraulic head (i.e., the pressure field of the system).

$$(2) \quad \frac{\partial h(x,y)}{\partial t} = \nabla \cdot (K(x,y)\nabla h)$$

Here, I presume that the pressure gradient is at a steady-state solution, so equation (2) becomes equation (3).

$$(3) \quad 0 = \nabla \cdot (K(x,y)\nabla h)$$

2.2.2. *Darcy's Law.* One can then calculate the flux of water, the specific discharge at a single point. The Darcy flux of water (i.e., the seepage velocity) q through a random conductivity field is described by Darcy's Law:

$$(4) \quad q(x,y) = -K(x,y)\nabla(h(x,y))$$

for K the conductivity, and h the hydraulic head. Note that K must be positive semi-definite. Since the fluid is flowing through a porous medium, the fluid exiting the medium is traveling through only a portion of the material (recall that the fluid travels through the void volume). Hence, the porosity of a medium affects the velocity experienced by both the fluid and the contaminant.

Thus, after solving equation (4) for the Darcy flow generated by the hydraulic head one can then calculate pore velocity v by dividing Darcy flux q by porosity n , as in equation (5).

$$(5) \quad v(x,y) = \frac{q(x,y)}{n}$$

The pore velocity is the velocity used in the Advection-Dispersion equation.

2.2.3. *The Advection-Dispersion Equation.* One can then solve the advection dispersion equation using the calculated pore velocity to model the contaminant transport problem over the random vector field. The advection-dispersion equation describes the flow of a contaminant through a saturated porous media. The same equation governs the spread of heat in space over a certain period of time. The spread of the contaminant in time is described by equation (6), for concentration of a certain contaminant c , dispersion coefficient D , and pore velocity of the fluid v .

$$(6) \quad \frac{\partial c(x,y)}{\partial t} = \nabla \cdot D\nabla c(x,y) - v(x,y) \cdot \nabla c(x,y)$$

Recall that here, the diffusive effect of the system is due to the random conductivity field which simulates the saturated porous media. The first term on the right of equation

(6) is the diffusive flux, the spread in the concentration due to the dispersion of the fluid. I presume that the dispersion coefficient is homogeneous, i.e., the spread of the contaminant is constant throughout the fluid. Note that D must be positive semidefinite. The second term on the right side describes the flow of the contaminant due to velocity of the system, imputed by the structure of the porous medium.

For homogeneous D , the advection-dispersion equation becomes:

$$(7) \quad \frac{\partial c(x,y)}{\partial t} = D\nabla^2 c(x,y) - v(x,y) \cdot \nabla c(x,y).$$

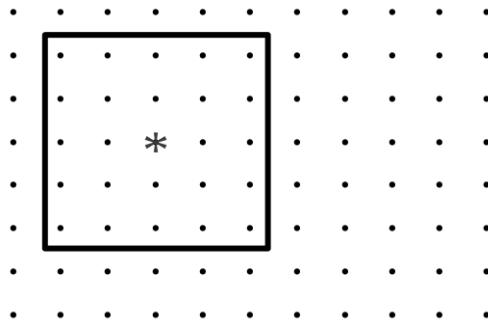
Solving equation (7) numerically yields the evolution of the contaminant profile throughout the simulated porous media.

3. NUMERICAL METHODS AND RESULTS

I created a code in MATLAB to solve the advection-dispersion equation over a random conductivity field. First, I generate a random conductivity field, then solve the steady-state diffusion equation for the hydraulic head. Then I solve for first the Darcy flux and secondly the pore velocity. Finally, I solve the advection-dispersion equation.

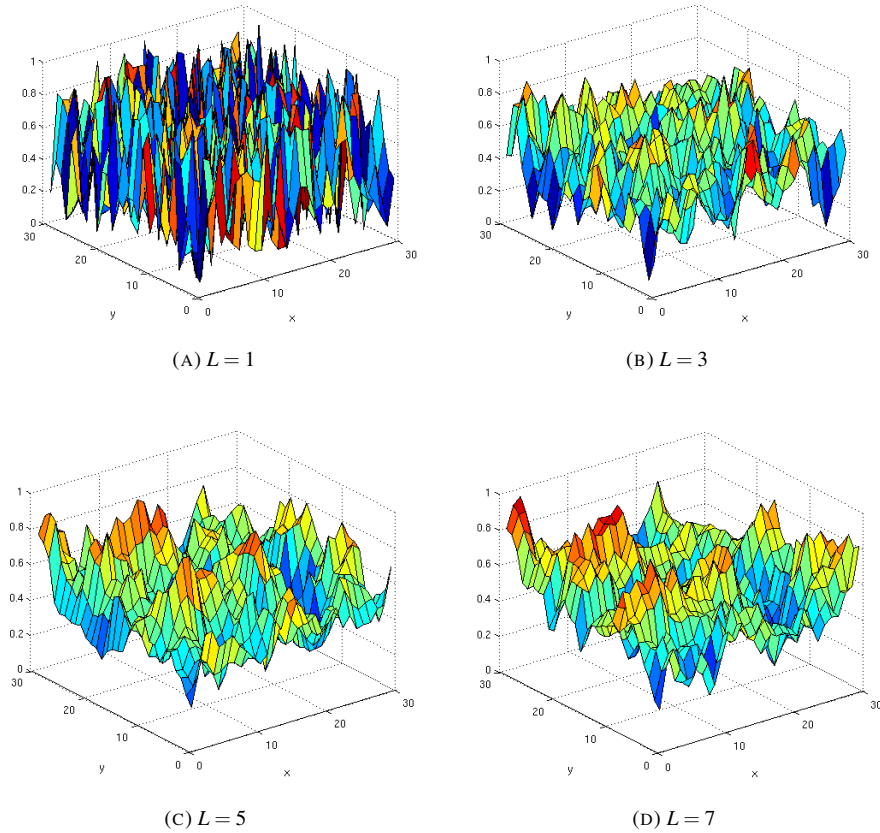
3.1. Random Conductivity Field. To create a random correlated conductivity field, I convolve random variables generated by the uniform distribution on $(0,1)$ with the identity function. Note that any other non-negative random variables would work just as well; the only restriction on K is that it be positive semi-definite. Since convolution with the identity function becomes addition, I take a window of size L , where L is always an odd number, add up the random variables contained in that window, and multiply by a scaling parameter. This scaled value is assigned as the conductivity value for the point at the center of the window. This creates a random, correlated field, normalized to the interval $(0,1)$, as pictured in Figure 1.

FIGURE 1. The underlying random vector field shown (of size 8×11 , each random variable denoted by \bullet) will create a random correlated conductivity field of size 4×7 . A window size of $L = 5$ sums the 25 random vectors contained in the window, creating the value of the conductivity field at the point labeled as $*$.



To generate a conductivity field of size F_x by F_y , I generate an underlying field of uniform distribution random variables, of size $F_x + L - 1$ by $F_y + L - 1$. The underlying field is of a larger size than the field generated due to the need for “ghost cells” beyond the range

FIGURE 2. Random correlated vector fields of size 30 by 30 generated by different window sizes, using the same underlying random vector field.



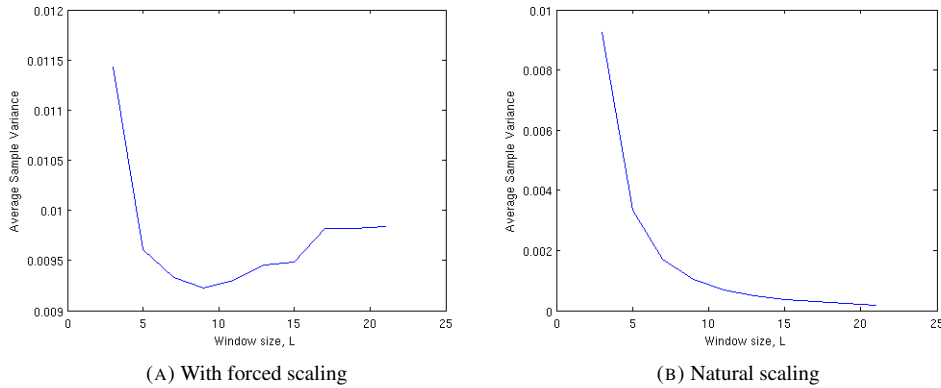
of the field. As the window travels over the entire underlying field, the random variables are included in multiple windows, which creates a correlated random field.

As shown in Figure 2, increasing the window size increases the correlation between the conductivity generated at each point. Quantitatively, running the random field generator for multiple iterations of a 1000 by 1000 point vector field and varying the window sizes used to generate the conductivity field shows the change in sample variance caused by the change in window size, as shown in Figure 3.

As seen in Figure 3, increasing the window size does decrease the sample variance. This is expected since larger window sizes correspond with a greater overlap of random variables in each window. In general, for a window size of L , two adjacent conductivity points will have an overlap of $L^2 - L$ underlying random variables. Hence, as L increases, the two generated conductivity points will be increasingly correlated.

3.1.1. *Scaling the Random Conductivity Field.* Because the conductivity field needs to be positive semi-definite, and because I want to be able to control the generated field, I experimented with different scaling parameters. Depending on whether I impose a “forced”

FIGURE 3. Average sample variance from 100 different random correlated vector fields of size 1000 by 1000 generated by odd window sizes varying from $L = 3$ to $L = 21$, with a forced scaling of generated field to between 0.05 and 0.95 and with a natural scaling of the field.



scaling condition or a “natural” scaling condition, either sample variance reaches a trough, or sample variance continues to decrease with increasing window size. When the forced scaling condition is imposed (i.e., the generated random correlated vector field is forced to have values between 0.05 and 0.95, inclusive), increasing the window size past $L=9$ actually slightly increases the sample variance, as shown in Figure 3. This is likely due to the artificial construction of the scaling; the field stretches to match the scaling parameters. If instead I scale the convolution by the inverse number of elements in the window, $1/L^2$, the generated field is now between 0 and 1 and the sample variance continues to decrease with increasing window size, as is expected. In addition, with the forced scaling condition, the average mean of the 100 different samples is not exactly 0.50, again due to the scaling parameters on the field pulling the random vectors away from the expected mean. When instead I use the natural scaling, the average sample means are very close the 0.50, the expected mean one would obtain when adding up N random variables uniformly distributed on $(0,1)$. However, with this natural scaling, the randomness of the process means that one has little control over the actual values the field takes.

3.2. Solving for the Steady State Hydraulic Flux. Once I have generated the random conductivity field, there are a few layers to solving the contaminant transport problem numerically. I first solve for the steady state solution of the diffusion equation to find a pressure field. Once the hydraulic gradient is found, I use Darcy’s Law to find the flux and then use porosity to calculate the pore velocity of the system. The pore velocities are then substituted into into the full advection-dispersion equation to numerically solve the contaminant transport problem.

The project involves the solution of two different PDEs. Standard methods for solving PDEs include finite differences, domain decomposition, volume conservative methods, and finite element methods. For this paper, I pursue the method of finite differences.

Because I want to generate an overall net flux in the y (horizontal) direction, I use constant boundaries on the left and right sides of my pressure equation, and use no flow boundaries on the top and bottom.

Once the problem has been discretized using finite differences, I can use an implicit solver, because I want to find the steady state solution to the diffusion equation over the random conductivity field. If the problem were not posed as finding the steady state solution, I would need to use a different method.

3.2.1. *Rewriting a Three Dimensional Problem as a Two Dimensional Problem.* To iterate the diffusion equation, note that one can rewrite the three dimensional system (two dimensions of space and one dimension of time) as a two dimensional system.

For example, a 4×4 matrix system \hat{H}

$$\hat{H} = \begin{pmatrix} \hat{h}_{1,1} & \hat{h}_{1,2} & \hat{h}_{1,3} & \hat{h}_{1,4} \\ \hat{h}_{2,1} & \hat{h}_{2,2} & \hat{h}_{2,3} & \hat{h}_{2,4} \\ \hat{h}_{3,1} & \hat{h}_{3,2} & \hat{h}_{3,3} & \hat{h}_{3,4} \\ \hat{h}_{4,1} & \hat{h}_{4,2} & \hat{h}_{4,3} & \hat{h}_{4,4} \end{pmatrix}$$

can be rewritten as the vector \mathbf{h} by stacking the columns on top of each other.

$$\mathbf{h} = (\hat{h}_{1,1} \ \hat{h}_{2,1} \ \hat{h}_{3,1} \ \hat{h}_{4,1} \ \hat{h}_{1,2} \ \hat{h}_{2,2} \ \dots \ \hat{h}_{1,4} \ \hat{h}_{2,4} \ \hat{h}_{3,4} \ \hat{h}_{4,4})^T$$

Renumbering the subscripts, one obtains the following vector \mathbf{h} :

$$\mathbf{h} = (h_1 \ h_2 \ h_3 \ h_4 \ h_5 \ h_6 \ \dots \ h_{13} \ h_{14} \ h_{15} \ h_{16})^T.$$

To evolve the diffusion equation, one must perform modular arithmetic on the vector \mathbf{h} , noting that each point is coupled to the points on the left and right, as well as to the points above and below. In the 4×4 example, the point directly to the left of point $\hat{h}_{2,2}$ is the point $\hat{h}_{2,1}$, corresponding to points h_6 and h_2 , respectively. In general, modular arithmetic yields that the point directly to the left of h_k corresponds to h_{k-n_x} , where n_x is the number of points in the x (vertical) direction of the system.

3.2.2. *A Simplified Example—The Diffusion Equation with Homogeneous K .* For the pressure $h(t, x, y)$ as a function of time and space, I have the diffusion equation in two dimensions, where K is the diffusion coefficient, assumed for this simplified example to be both isotropic and homogeneous:

$$(8) \quad \frac{\partial h}{\partial t} = K \left(\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} \right).$$

Using centralized differences with time stepping indicated by superscript (m) and space stepping in x, y indicated by subscripts i, j respectively, one obtains a discretized version of the advection diffusion equation, as seen in equation (9).

$$(9) \quad \frac{h_{i,j}^{(m+1)} - h_{i,j}^{(m)}}{\Delta t} = K \left(\frac{h_{i+1,j}^{(m+1)} - 2h_{i,j}^{(m+1)} + h_{i-1,j}^{(m+1)}}{(\Delta x)^2} + \frac{h_{i,j+1}^{(m+1)} - 2h_{i,j}^{(m+1)} + h_{i,j-1}^{(m+1)}}{(\Delta y)^2} \right).$$

Note that the equation above is fully implicit. Solving for the current time step (m) , obtains the formula:

$$(10) \quad h_{i,j}^{(m)} = h_{i,j}^{(m+1)} - K \Delta t \left(\frac{h_{i+1,j}^{(m+1)} - 2h_{i,j}^{(m+1)} + h_{i-1,j}^{(m+1)}}{(\Delta x)^2} + \frac{h_{i,j+1}^{(m+1)} - 2h_{i,j}^{(m+1)} + h_{i,j-1}^{(m+1)}}{(\Delta y)^2} \right).$$

To quickly solve for the steady-state pressure field using $h_t = \nabla \cdot (K \nabla h) \doteq 0$, I write the discretized equation into matrix form, then use the implicit method of Backward Euler to solve numerically with the condition that $|\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)}| < \text{TOL}$, for some tolerance level TOL. Using inspiration from Numerical Recipes in C, the discretized diffusion equation can then be placed in matrix form [6]. The matrix couples all of the points together in a

then sum the matrices together to create one matrix that evolves the equation. I then use Backward Euler to solve, as in the simplified example above.

3.2.4. *General Methods for Finding the Hydraulic Head.* To improve speed of the code, one can make use of the sparsity of the matrix. A few applications of an implicit method such as Backward Euler obtains the pressure matrix for the random vector field. Note that using an implicit method means that the time step can be very large. This allows rapid calculation of the pressure field (i.e., the hydraulic head).

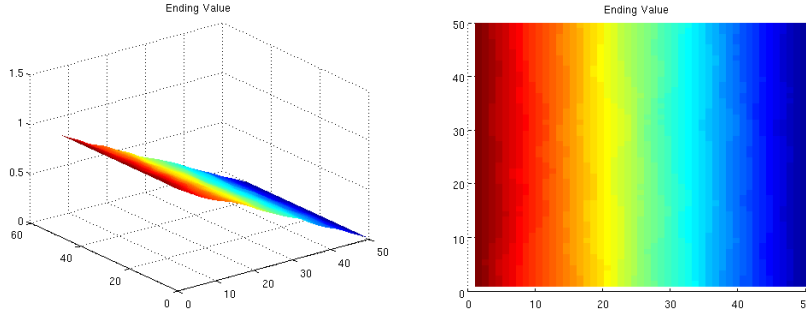


FIGURE 5. Pressure field generated for 50×50 grid using window $L=3$, left boundary fixed at 1.0, right boundary fixed at 0.0 and no-flow conditions top and bottom. $\Delta x = \Delta y = 0.01$. Two views shown.

It is simple to calculate the hydraulic flux and then the pore velocity, according to equation (4) and equation (5). Due to the boundary conditions, with a constant pressure at the left edge of the system, the pore velocity is dominated by that in the y -direction. Finally, I can solve the advection-dispersion equation.

3.3. **Solving the Contaminant Transport Problem.** Similarly to the diffusion equation, I can discretize the advection-dispersion equation (repeated below), but using an explicit method since there is no longer a steady-state condition.

$$\frac{\partial c(x,y)}{\partial t} = D\nabla^2 c(x,y) - v(x,y) \cdot \nabla c(x,y)$$

Recall that D the dispersion coefficient is homogeneous throughout the field. Using explicit finite differences, with current time step (m), the advection-dispersion equation becomes

$$\frac{c_{i,j}^{(m+1)} - c_{i,j}^{(m)}}{\Delta t} = D \left(\frac{c_{i+1,j}^{(m)} - 2c_{i,j}^{(m)} + c_{i-1,j}^{(m)}}{(\Delta x)^2} + \frac{c_{i,j+1}^{(m)} - 2c_{i,j}^{(m)} + c_{i,j-1}^{(m)}}{(\Delta y)^2} \right) - v_{x,i,j}^{(m)} c_{i,j}^{(m)} - v_{y,i,j}^{(m)} c_{i,j}^{(m)}.$$

Solving for time step ($m+1$), I obtain the formula:

$$c_{i,j}^{(m+1)} = c_{i,j}^{(m)} + \Delta t \left(D \left(\frac{c_{i+1,j}^{(m)} - 2c_{i,j}^{(m)} + c_{i-1,j}^{(m)}}{(\Delta x)^2} + \frac{c_{i,j+1}^{(m)} - 2c_{i,j}^{(m)} + c_{i,j-1}^{(m)}}{(\Delta y)^2} \right) - v_{x,i,j}^{(m)} c_{i,j}^{(m)} - v_{y,i,j}^{(m)} c_{i,j}^{(m)} \right).$$

Here, D the dispersion coefficient is assumed to be homogeneous, since the dispersion of the contaminant should be the same throughout the fluid. The non-uniform profile of the contaminant will instead be created by the velocity field.

To evolve the advection dispersion-equation at each time step, I run it through a series of for-loops to calculate the concentration of the contaminant at each cell. Now, since the equation is no longer solving for a steady state, one cannot use Backward Euler to solve the equation numerically. Instead, I use a predictor corrector method to numerically solve the advection-dispersion equation.

I choose begin with a few iterations of Forward Euler, then proceed with Adams-Bashforth 2, Adams-Moulton 3, a linear multistep method [2]. Let $f = f(t, x, y)$ be the advection-dispersion equation, and y_i the concentration of contaminant at time step i . Given initial values f_0, f_1, y_1 , for each iteration one has:

$$\begin{aligned} y_2 &= y_1 + \frac{h}{2}(3f_1 - f_0) \\ y_3 &= y_1 + \frac{h}{2}(5f_2 + 8f_1 - f_0) \end{aligned}$$

As long as the time step is small enough, the equation behaves well. For too large of a time-step, the numerical solution begins oscillating.

Running the code with $\Delta t = 1e - 8$ on a 50×50 grid through $t = 20.00e - 5$, yields the following numerical results, shown in Figure 6. Despite the inhomogeneous velocity field, the evolution of the system closely resembles the Gaussian distribution expected from a point source contaminant. With the other parameter combinations I tried, it was similarly difficult to qualitatively tell the difference between a standard Gaussian and the numerical solution profile. While I am confident the correct parameter set can be found that will properly show off the inhomogeneity, more research needs to be done.

4. DISCUSSION

Using an underlying vector field of identical, uniformly distributed random variables one can implement a “natural” scaling to control both the average conductivity and the correlation of the variables, or implement a “forced” scaling to control the minimum and maximum conductivity, with some control over the average conductivity. However, using a forced scaling to control the minimum and maximum of the conductivity field wreaks havoc with the correlation of the data points, and instead of the expected drop in the average sample variance, one actually observes growth past a certain window size. The best method seems to be controlling the average conductivity by using a single scaling coefficient to change the population mean, and then to control the correlation of the conductivity at each point by changing the window size used in the convolution. One could also scale by a coefficient and then add a constant; this would have the same effect.

It appears that using the methods described above, one can qualitatively solve the contaminant transport problem over a random, correlated conductivity field. Solving the pressure field using Backward Euler to find the steady state is quite efficient. This is a well-posed problem with steady state conditions.

Unfortunately, solving the advection-dispersion equation is more difficult. After running the code several times with different parameters, it is apparent that the method used is not volume conservative. While qualitatively the solution appears correct, summing over the mass in each cell shows that the total mass is non-constant. Comparison with the exact

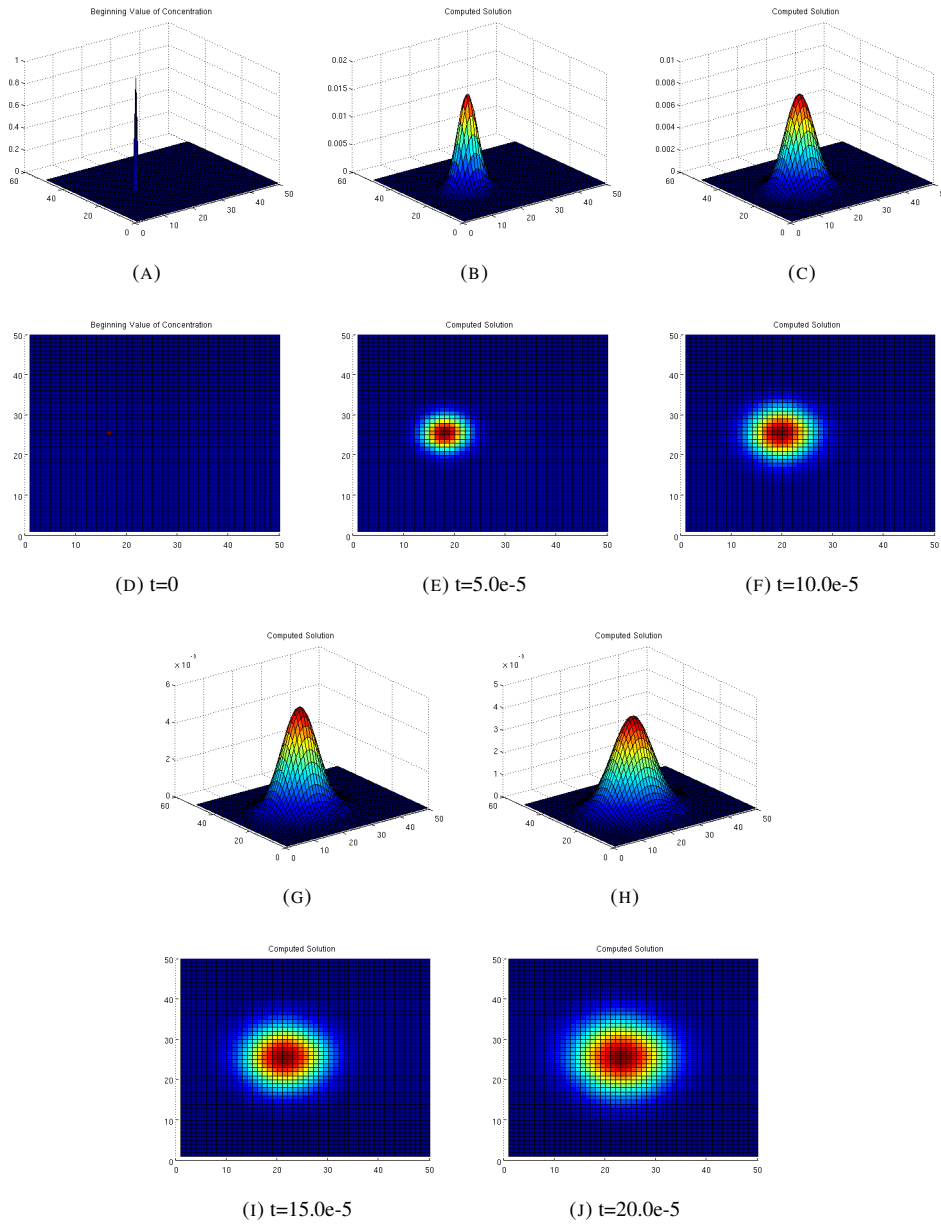


FIGURE 6. Evolution of the advection-dispersion equation in time, on a 50×50 grid with dispersion coefficient of $D = 0.1$. Initial condition of a single point source implemented at $t=0$, over the pressure field shown in Figure 5. $\Delta x = \Delta y = 0.01$, $\Delta t = 1.00e - 9$. The evolution looks very similar to that of a Gaussian, but is slightly anisotropic. Two views shown for each time step.

solution of a point source (a well-known Gaussian) shows that while the code yields quantitatively correct results and approximately tracks the general movement of the contaminant, the mass at each cell varies somewhat from the exact solution.

5. FUTURE RESEARCH DIRECTIONS

The current method used to discretize the advection-dispersion equation is finite differences. Unfortunately, this is not a volume-conservative method, and this particular problem is very concerned with following the exact volume of the contaminant. The non-constant volume of the system is perhaps exacerbated by testing the code on a point mass of a contaminant, which is very poorly conditioned. However, to address the non-constant volume issue, the next step of this research should be to implement a volume conservative method.

It would be interesting to further study the increase in correlation of average sample variance with increasing window size, perhaps by calculating fractal dimensions of the generated random conductivity field. More investigation into possible control over this random process would also be interesting—to what extent can one control or bound the conductivity field without imposing unfortunate artifacts such as the increase in variance after a certain window size?

A traditional method for dealing with the uncertainty in pore space structure is to use Monte-Carlo simulations, repeating the procedure several times over to generate an average. However, such simulations are computationally expensive. One could improve on the efficiency of such models by using a spatial averaging process to create a simplified model, using the traditional Monte-Carlo simulations to validate the results.

6. CONCLUDING REMARKS

The end goal is to create a computationally efficient, yet still effective model of the failure of groundwater remediation measures, by averaging the flow of the contaminant over space rather than calculating the flow through every single pore or using Monte-Carlo simulations. Currently the project is in the early stages.

Once completed, the resulting general code will allow scientists to investigate the best type of groundwater remediation based on parameters from each spill site. While by no means will this research eliminate future tragedies such as Love Canal, it will perhaps help find a chink in the armor of this enormous problem.

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APPENDIX A

Porosities of common media [7].

Medium	Porosity, n
Clay	0.34 to 0.57
Granite	0.001
Gravel, fine	0.25 to 0.38
Gravel, coarse	0.24 to 0.36
Gravel and sand	0.20 to 0.35
Sand, uniform	0.30 to 0.40
Soils	0.50 to 0.60

APPENDIX B

I apply the boundary conditions by solving equations for each point, adding “ghost cells” where necessary. For example, the diffusion equation applied in the x (vertical) direction to the pressure at point $h_{1,2}$ from time step (m) to time step $(m+1)$ is described by the following equation:

$$\frac{h_{1,2}^{(m+1)} - h_{1,2}^{(m)}}{\Delta t} = \frac{h_{0,2}^{(m+1)} - 2h_{1,2}^{(m+1)} + h_{2,2}^{(m+1)}}{(\Delta x)^2};$$

Note that the cell $h_{0,2}$ is not actually part of the system, and hence, one does not know the value at that point. One uses the boundary conditions to solve for the value of $h_{0,2}$. Due to the no-flow boundary conditions at the top and bottom, the velocity condition in the x direction at point $h_{1,2}$ is described by the following equation:

$$\frac{h_{2,2} - h_{0,2}}{2\Delta x} = 0,$$

whence $h_{0,2} = h_{2,2}$. Then the diffusion equation in the x direction at this point becomes

$$\begin{aligned} \frac{h_{1,2}^{(m+1)} - h_{1,2}^{(m)}}{\Delta t} &= \frac{h_{0,2}^{(m+1)} - 2h_{1,2}^{(m+1)} + h_{2,2}^{(m+1)}}{(\Delta x)^2} \\ &= \frac{2h_{2,2}^{(m+1)} - 2h_{1,2}^{(m+1)}}{(\Delta x)^2}. \end{aligned}$$

Hence, the no-flow boundary conditions at the top and bottom of the system account for the values of 2 found in the superdiagonal and subdiagonal of matrix \mathbf{A} in Figure 4. Note that while from the equation above it appears the diagonal coefficient should be -2, it is actually -4 since it diagonal elements experience diffusion in both the horizontal and vertical directions.