COMSOL Modeling of Groundwater Flow and Contaminant Transport in Two-Dimensional Geometries With Heterogeneities

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Abstract: The Delmarva Peninsula is located on the East Coast of the United States, between the Chesapeake Bay and Atlantic Ocean. Industrial farming in the Delmarva Peninsula leads to levels of nutrients, in particular nitrogen, which grossly exceed natural levels. Excess nitrogen reaches the freshwater streams of the peninsula, which then flows to the Chesapeake Bay. The presence of extreme levels of nitrogen greatly impairs the health of the bay, 48% of a streams nitrogen load has been discharged from groundwater.

The surficial aquifer geometry in this area is marked by significant geological structures: a general sloping confining layer, angled toward the ocean with unconfined surface strata of sand and clay. The aquifer contains groundwater that flows to the streams of the peninsula. The clay strata are sloping banks three-to-four meters thick, through which groundwater flows much more slowly than the sand strata. We use the software package COMSOL Multiphysics 4.1 to quantify how water residence times change due to heterogeneities within two-dimensional cross-sections by creating a model representative of the region.

We find that variation in clay strata affects flow paths. A phreatic divide is the point on the surface that delineates the output river for recharge. The presence of clay banks within the aquifer shifts the location of the phreatic divide. Furthermore, the hydraulic pressure head increases with the presence of clay strata shortening the length of time water and nutrients spend within the aquifer.

Key words: Groundwater flow, nutrient transport, Delmarva Peninsula, Environmental Systems.

1 Introduction

Groundwater contributes an large portion of stream flow and subsequently nutrients to rivers in the Delmarva Peninsula. The region is large and complex geologically. Underlying clay heterogeneities disrupt the uniformity within the aquifer, creating dynamics which are very difficult to quantify in their entirety. The purpose of this project is to determine general rules about how clay heterogeneities affect both the movement of groundwater within the aquifer and the transport of nutrient concentration to rivers. A general assessment is needed to quantify the relative importance of subsurface heterogeneity in affecting patterns of nutrient transport.

1.1 Geometry

To represent the Delmarva region, a general aquifer cross-section between two rivers is created, Figure 1. The important features of the region are then incorporated into the aquifer. These features include the long and thin nature of the aquifer, the width is forty-four times that of the height, and the angled impermeable aquitard. In the general aquifer there are two simulated rivers, these are used to quantify how water flows to each river depending on heterogeneities within the aquifer and the angle of the impenetrable bottom.

To this general aquifer clay heterogeneities are added; this is seen in Figure 2. The clay heterogeneities are three meters thick and are of the same angle. To understand how these heterogeneities affect groundwater flow we will observe four representative geometries for clay placement. The het-

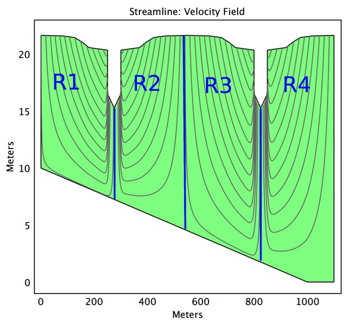


Figure 1: Representative geometry with labeled regions.

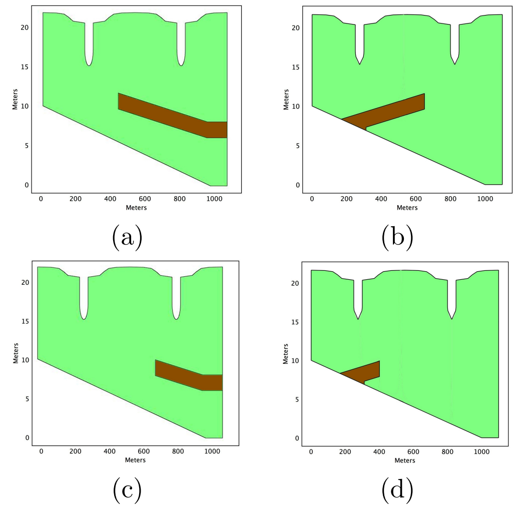


Figure 2: Geometries with heterogeneities, occurring: after the divide from the right, (a), and from the left, (b), before the divide from the right, (c) and from the left, (d). Note: the scale of x and y are not the same.

erogeneities are placed either from the left or right of the bank. When heterogeneities are placed from the right they are approximately parallel to the impenetrable bottom, placed on the left heterogeneities create a bottom which is no longer parallel to the bottom.

There are two natural (phreatic) divides which occur within the aquifer; under the stream and between two streams. Without the presence of heterogeneities the phreatic divide of the representative geometry occurs at $x = 537$ meters. The phreatic divide is used to dictate the length of the clay bank. Heterogeneities are either "long", their end terminates after the divide or "short", their end terminates before the phreatic divide.

The three natural divides creates four flow regions in our geometry which we will refer to to compare the changes within the aquifer due to heterogeneities. These regions are labeled in Figure 1.

1.2 Simulations

To analyze the effects of clay heterogeneities in the representative aquifer two coupled partial differential equations will be applied to the geometries. These are assigned using Mathematics, PDE Interfaces: **Coefficient Form, PDE** and are of two study subset types, Stationary and Time Dependent. The first PDE is stationary and finds the solution to the Darcy velocity; it will be analyzed and discussed in Section 2. This solution gives rise to the direction which recharge takes, and which river this water flows to. The second PDE is time dependent and finds the solution to the advection diffusion equation; it will be applied to quantify the time at which nutrients reach the river beds and discussed in Section 3.

2 Stationary Flow

Darcy's flux in two-dimensions prescribed to the geometry using in the following steady state equation

$$q = -\overline{K}\nabla\phi, \tag{2.1}$$

where ϕ is the hydraulic pressure head, measurement of water pressure above a geodetic datum, the reference datum is typically an arbitrary horizontal surface, for large scale models sea level is used [2], it has a dimension of length. $\overline{K}$ is the hydraulic conductivity for a particular media, a parameter dependent on two properties form the fluid, its viscosity and density, and on properties from the medium such as intrinsic permeability which is measured by the particle diameters in the porous medium. The aquifer material consists of sandy loam, with a saturated hydraulic conductivity of approximately $\overline{K} = 10^{-4}$ and clay heterogeneities, which have a saturated hydraulic conductivity of $\overline{K} = 10^{-9}$ [6]. These are easily assigned to the system by defining them in Global Definitions.

2.1 Groundwater Velocity

The Darcy flux is not the velocity of the fluid within the media. This pore velocity is related to the Darcy flux by the porosity, n, of the medium.

Porosity is dependent upon the medium, and so, $n = 0.35$ for sand, and $n = 0.60$ for clay. Thus the pore velocity of a groundwater in an aquifer is described by equation (2.2). Darcy velocity is the common term which couples the two PDEs in the system.

$$v = \frac{q}{n} = -\frac{\overline{K}}{n}\nabla\phi \tag{2.2}$$

2.2 Hydraulic Pressure Head

It has been shown as an aquifer deepens hydraulic pressure is lowered, since fluid flows from high to low pressure, a higher percentage of groundwater will flow in the deeper aquifer [7]. Therefore, without the presence of heterogeneities the average length of flow paths increase in each subsequent region. This changes with the addition of clay heterogeneities.

When large clay heterogeneities are added to the aquifer changes in hydraulic pressure head occur, as seen in Figure 3. Pressure is lowest under rivers and highest further away. Heterogeneities increase the amount of hydraulic pressure head within the regions they are located, in other words deeper regions have been effectively truncated. This increase of pressure is most prevalent in between the two rivers, most pronounced are the cases where the heterogeneity protrudes past the divide. In these two cases pressure levels are similar to, if not higher than, those seen in Region 1 in Regions 2 and 3.

Pressure changes also shift the phreatic divide. Since fluid flows from high to low pressure, a higher percentage groundwater will flow in deeper parts of the aquifer. Therefore, the divide shifts to the right when the heterogeneity protrudes from the right.

Divide lines are important for two reasons: they delineate to which river water from the surface will flow and they also correspond to the part of the domain where the longest streamlines occur. The longest flow lines are directly next to the phreatic divide, and the shortest streamlines are furthest from the phreatic divide and nearest each river. The length of the streamlines are important as they dictate the residence time, or time water stays within the aquifer. The longest flow lines correspond to the longest residence times [3, 7].

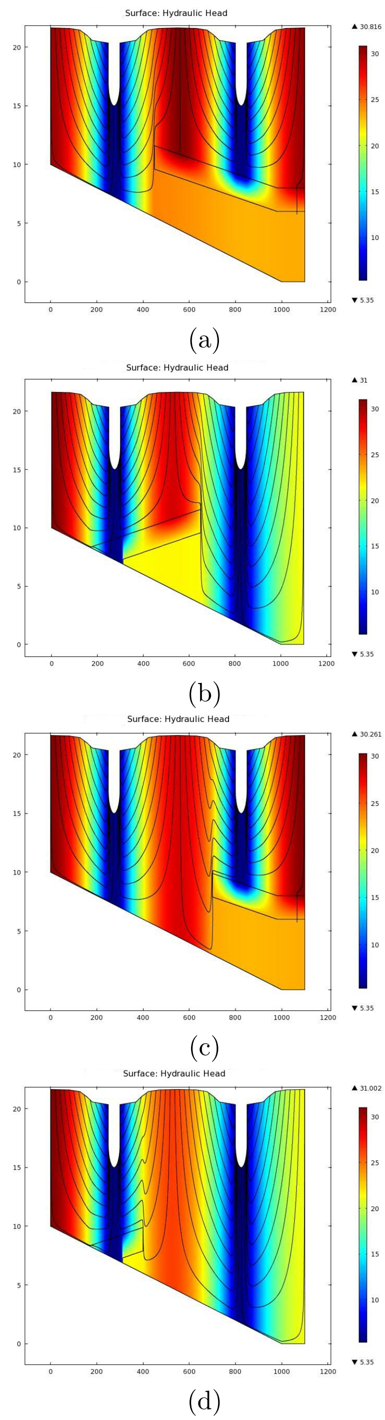


Figure 3: Hydraulic pressure head as as solved within the geometry for each heterogeneous case.

3 Transient Flow

Nutrient transport within the aquifer is facilitated by both diffusion and advection, which is described by the following PDE

$$\frac{\partial C}{\partial t} = -\nabla \cdot (-D\,\nabla C + vC), \tag{3.1}$$

where C is the concentration of the nutrient at a given time, D is the diffusion coefficient derived in Section 3.1 and v is Darcy's velocity at a certain point in space, Equation (2.2).

3.1 The Coefficient of Dispersion

In multiple dimensions, dispersivity can be explained by two constants, transverse dispersivity, α_T, and longitudinal dispersivity, α_L. Longitudinal dispersivity is the dispersion of particles which occurs along the horizontal plane in the field, and transverse dispersivity describes derspersion not along this plane. Dispersion values for transverse dispersivity are generally much smaller than that of longitudinal. For this study, we will let $\alpha_T = 0.005$, and $\alpha_L = 0.5$ [1, 4]. In component form we define diffusion using longitudinal and transverse dispersivity in the following way:

$$D_{ii} = \alpha_L \frac{v_i^2}{||v||} + \alpha_T \sum_j \frac{v_j^2}{||v||} + D_m$$

$$D_{ij} = D_{ji} = (\alpha_L - \alpha_T)\frac{v_i v_j}{||v||}$$

We have normalized the velocity components using the Euclidean norm. Thus we can create our two-dimensional diffusion matrix as [5]

$$D = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22}, \end{bmatrix}$$

with

$$D_{11} = (\alpha_T v_2^2 + \alpha_L v_1^2)/\overline{v} + D_m,$$

$$D_{22} = (\alpha_T v_1^2 + \alpha_L v_2^2)/\overline{v} + D_m,$$

$$D_{12} = D_{21} = (\alpha_L - \alpha_T) v_1 v_2/\overline{v},$$

and the molar diffusion coefficient $D_m = 1.34 \times 10^{-9}$ cm^2/s is considered to be a constant.

3.2 Initial Conditions & Run Time

The initial condition is zero, assuming an initially clean environment. This simulates conditions before industrialized farming began. To observe long term effects of industrialized farming, we will carry our time frame to over 70 years.

3.3 Fertilizer Distribution

Fertilizer is applied to the surface once a year starting at the beginning of the growing season, and we assume that for the subsequent three months of the year it leaches into the ground. This can be simulated with a cycling step function applied to the top boundary of the model.

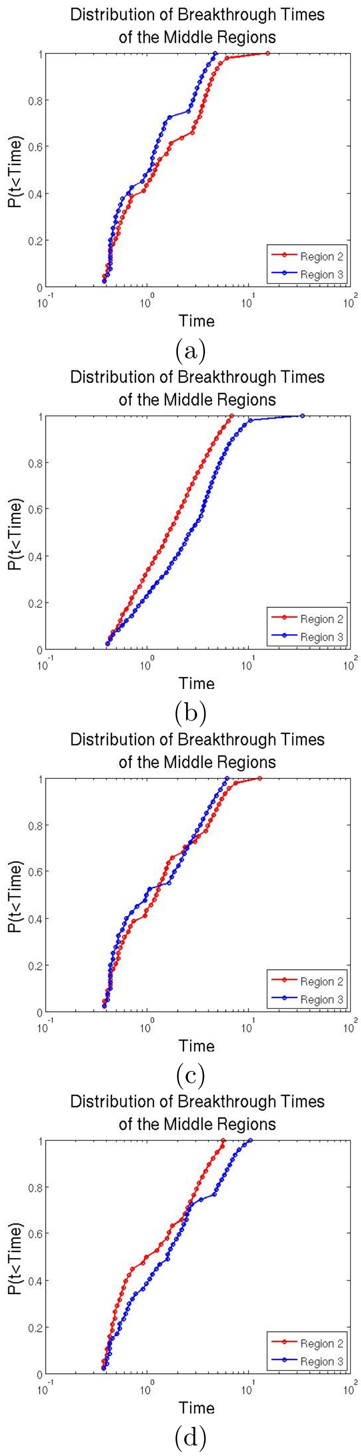
The COMSOL function **flc2hs** is used to create this cycling function. By then applying a modulus over time the equation will cycle from 0 to 1 for 90 days every year. In order to reduce runtime the solver time step is set to be every thirty days over the seventy years. Additionally, due to the extremely small window in which the fertilizer occurs strict time stepping is implemented, in order to catch the fertilizer distribution each year.

3.4 Breakthrough Timing

Since velocity is directly proportional to pressure head, as seen in Equation (2.2), changes in pressure effect nutrient transport. Fertilizer is distributed along the boundary of Regions 2 and 3. Nutrient movement within these two regions is of greatest interest due to the dynamical nature of the phreatic divide.

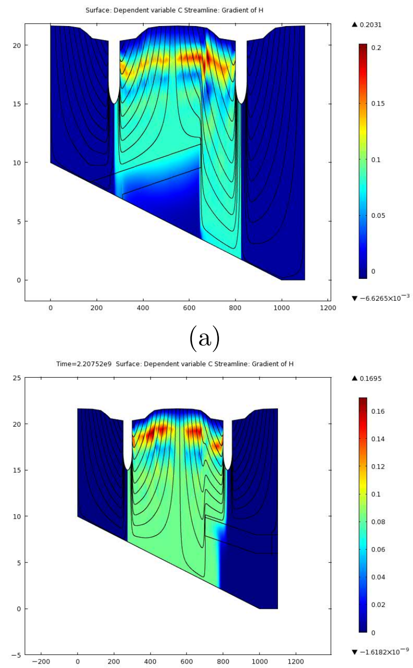
Concentration levels are post-processed by exporting concentration levels across all time on cutpoints along the boundary of each river. The cutpoints are the end points associated with 200 flow lines spaced evenly across the water table and occurring with the same starting location for each geometry. Nutrient breakthrough times are measured by finding the first time which concentration levels along the river boundary are above a certain threshold, $C_{threshold}$. We take $C_{threshold} = 0.001$, or 0.1% of the released nutrient load. Figure 4 displays the frequency distributions of the five cases.

Without heterogeneities Region 2 would have consistently faster breakthrough times than Region 3 [7]. This relationship changes with the presence of heterogeneities. Most noticeably when the heterogeneity protrudes from the right and terminates



(a) (b) (c) (d)

Figure 4: Breakthrough frequency plots for heterogeneous cases, (a) after the divide on the right, (b) after the divide on the left (c) before the divide from the right, and (d) before the divide from the left.



(a) (b)

Figure 5: Concentration within the aquifer after 70 years of fertilization

after the divide, in this case Region 3 is consistently faster than Region 2. Similarly, when he heterogeneity protrudes from the right and terminates before the divide, by the 75^{th}, quantile Region 3 is consistently faster than Region 2. In both these cases, the area which makes up Region 3 has been significantly lessened, there is a lager percentage of short flow paths.

It is important to note, the longest breakthrough times are never realized as the simulation runs for only seventy years. A small percentage of flow paths enter into clay banks and take centuries to exit the system. Others are so lengthened that they take decades to exit the system.

3.5 Nutrients Within the Aquifer

Figure 5 gives a good qualitative idea of how nutrients have moved and collected within the aquifer. Both (a) and (b) show a band of fertilizer, depicted in red, from the last input. The fertilizer input from the previous year can also still be seen in a lighter band at approximately $x = 15$. Fertilizer is applied equally across the water table, any changes to a profile which resembles the water table can be attributed to the flow path changes due to clay heterogeneities In Figure 5 (a) concentrations along flow lines which interact with the end of the heterogeneity, creating a region of higher concentration every year. It can also be seen that concentration levels along longer streamlines have reached a steady state, to a level below 0.01.

We have shown that flow paths enter clay banks, taking centuries to return to the river. Nutrients are carried along these flow paths and collect under clay heterogeneities. It is not in the scope of this project to measure the levels of nutrient concentration after centuries of yearly farming, but it is clear that nutrients will continue to build under the heterogeneity, as seen in Figure 5.

4 Conclusions

Flow dynamics and nutrient transport within the aquifer can be attributed to many factors. The conditions which drive flow direction and nutrient transport are: depth of the underlying aquifer, phreatic divide and placement and length of clay heterogeneities. Each of these factors influence how groundwater reaches a stream and the length of time nutrients take to reach a stream.

Heterogeneities change these dynamics within the aquifer. They change the pressure within the aquifer which changes velocity and residence times. It is clear that knowledge of when and where a heterogeneity exists within the aquifer is extremely important. The most important aspect of the dynamical system is the phreatic divide. A heterogeneity which protrudes from the shallow side (the left) will move the divide further to the middle of the two rivers. This means more flow paths will reach one river than the other, and therefore more nitrogen, if it is applied across the entire domain.

It is important to understand how placement of farmland on the water table will effect eventual nutrient levels in nearby streams. As stated above, the factors in nutrient flow to neighboring rivers are streamline divide and residence time. Both of these are effected by large clay heterogeneities. Long streamlines take a longer amount of time to deliver nutrient concentrations to a stream.

In conclusion, it is clear that heterogeneities change the dynamics within the aquifer, changing flow velocity and phreatic divides. This changes the amounts of nutrients which flow to the rivers. It is important to understand how these sample geometries are affected so that similar profiles can be found in the real landscape. These results can be used as a general framework for the large complicated landscape.

Acknowledgments

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