USING GMS TO DEVELOP A MODFLOW MODEL TO TRACK PARTICLES ASSOCIATED WITH SLURRY INJECTION[1]

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Abstract. An environmental issue concerns the fate and transport of contaminants that involve the injection of coal slurry into voids of abandoned underground West Virginia coal mines. Mines in the Pocahontas No.3 and No.4 coal seams in McDowell County have been injected with coal slurry for decades. This project describes how the Office of Surface Mining Reclamation and Enforcement's, National Technical Innovation and Professional Services Program software applications can model particles through complex flow paths using EMS-I Groundwater Modeling System 6.0 (GMS). A conceptual model approach was created using Geographical Information System (GIS) objects, including points, arcs, and polygons. The conceptual model was constructed independently of a grid or mesh and reflects the area sources/sinks and boundary conditions. The model was fitted with a grid to provide a relationship between the data and the geospatial model. The GMS graphical interface to the groundwater application MODFLOW was used to create a flow path. Contaminants in groundwater can be addressed using groundwater flow models and particle tracking. MODPATH is a particle tracking code that was developed by the United States Geological Survey (U.S.G.S.) and used in conjunction with MODFLOW. Using a flow field computed by MODFLOW, MODPATH can track a set of fictitious particles to simulate the movement of contaminants starting from user-defined locations. It is important to note the model includes many hydrological assumptions that were necessary in developing the model. The GMS model is being developed and used to better understand the possible flow path of slurry injectate to residential water wells, as well as determining how to better protect wells in source water areas.

Additional Key Words: MODPATH, GIS, mine, voids

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INTRODUCTION

A scenario of a hydrogeological study of the migration of coal slurry from an injection well into the groundwater or surface waters was simulated using a four layer site specific groundwater flow model. The model was constructed using the U.S. Geological Survey groundwater flow model, MODFLOW to simulate a flow direction of coal slurry injected into the subsurface. One of the factors of groundwater contamination is its long term nature. Contaminants in groundwater can be evaluated using groundwater flow models and particle tracking. MODPATH is a particle tracking code that is used in conjunction with MODFLOW. Using a flow field computed by MODFLOW, it is then possible to use MODPATH to track a set of fictitious particles to simulate the movement of contaminants starting from user-defined locations.

In studying the groundwater flow system a conceptual model was developed to define the individual layers in the model. A steady-state, three-dimensional, finite-difference groundwater flow model was developed to simulate the flow pattern of the aquifer system that encapsulates the injection well. The method of injecting coal slurry into old abandoned underground mines has been recorded since early 1980s. Coal slurry consists of solid and liquid waste and by-product of the coal mining and preparation processes.

The state of West Virginia received UIC (Underground Injection Control) primacy from EPA in 1984. In June 1999 the UIC program began issuing UIC permits to mining facilities disposing of mine waste into coal seam mine voids. Legislative Rules, Department of Environmental Protection Office of Water Resources Series 58, Groundwater Protection Rule establishes a series of practices which must be followed by any person who owns or operates facilities or conducts activities subject to the provisions of W.Va. Code §22-12-1 et seq. and is subject to regulation by the Department of Environmental Protection's Office of Waste Management or Office of Water Resources.

All applications must include identified receiving coal seam voids, maps showing all mine workings within a one-mile radius, height of coal void, and thickness of barriers as well as the effects on the hydrologic regime including the location and description of permanent monitoring wells or monitoring stations, gradient of the mine from the backfill area, description of the stratum underlying the mined coal, and source and quality of the refuse.

The Pocahontas No. 3 coal seam in McDowell County, West Virginia has been injected with coal slurry that is potentially migrating through unknown flow paths down gradient. This model describes how such a situation could be modeled using GMS. The location of the regional study area is shown in (Figure 1).

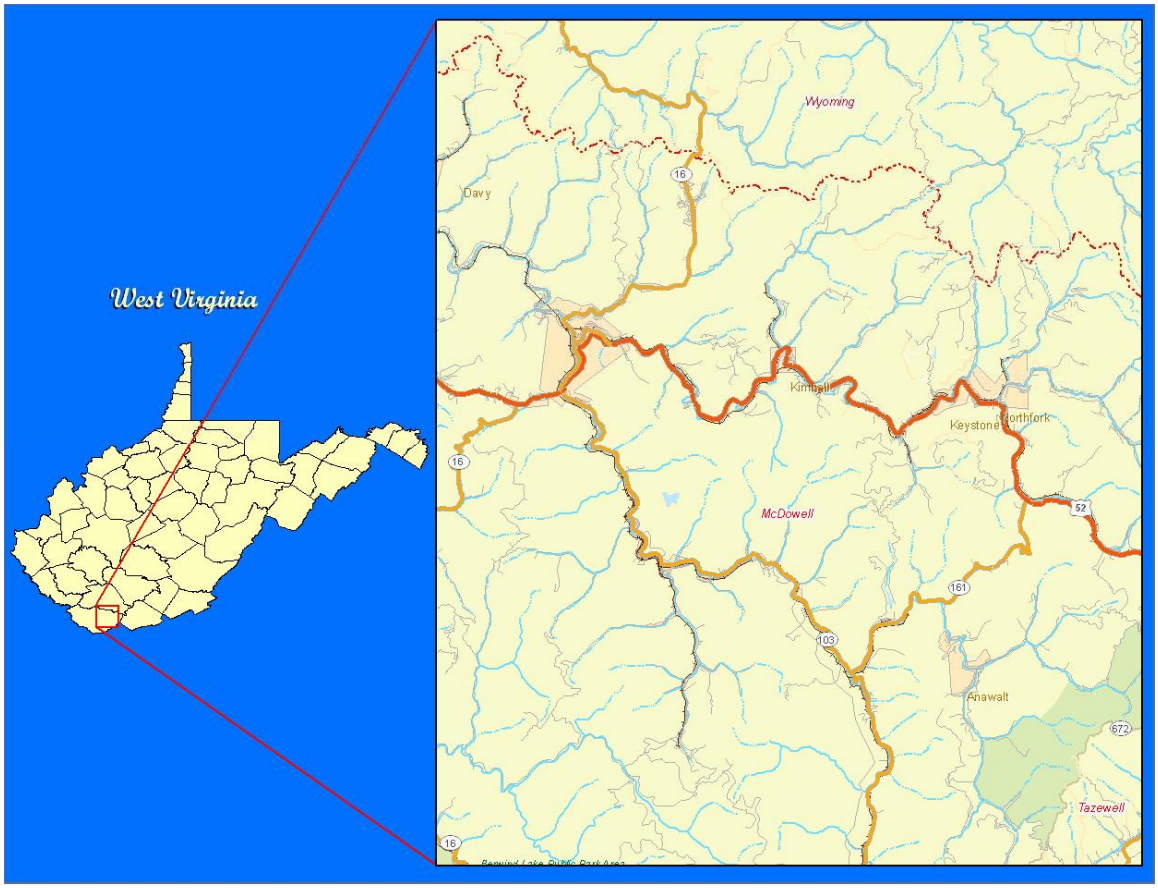


Figure 1. Location map of the study area

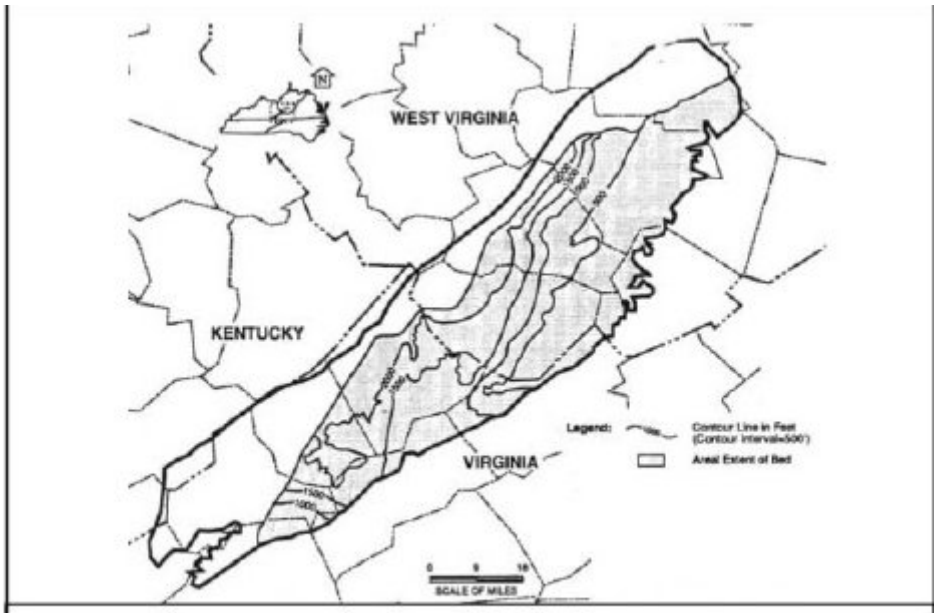
PHYSICAL SETTING

The Pocahontas Formation directly overlies the Mississippian Bluestone Formation, and was deposited in an unstable basin that was rapidly subsiding to the southeast (Kelafant et al., 1988). This is reflected in the thickness of the formation, which is thickest in the southeast and thins to the northwest. It also thins to the south and west due to erosion caused by the basal sandstone member of the overlying New River/Lee Formation (Kelafant et al., 1988). The Pocahontas Formation reaches its maximum thickness of 750 feet near Pocahontas, Virginia (Kelafant et al., 1988). The formation consists mostly of massively bedded, medium-grained subgraywacke,

which can be locally conglomeratic (Kelafant, 1988). Gray siltstones and shales are interbedded within the sandstone (subgraywacke) unit, and coal seams comprise about two percent of the total thickness of the Pocahontas Formation (Kelafant et al., 1988).

The Pocahontas No. 3 coal seam ranges in depth from outcrop along the northeastern edge of the basin to about 2,500 feet, with a thickness ranging up to seven feet (Kelafant et al., 1988). Depths to the Pocahontas No. 4 coal seam are somewhat similar to those for the Pocahontas No. 3 coal seam, as the No. 4 seam overlies the No. 3 seam by roughly 30 to 100 feet. The thickness of the No. 3 coal seam varies, with a maximum of approximately seven feet (Kelafant et al., 1988). The Fire Creek/Lower Horsepen coalbed ranges in depth from roughly 500 feet over half of its area, to a maximum depth of approximately 1,500 feet, with a maximum thickness of roughly six feet (Kelafant et al., 1988).

The Pocahontas Formation is restricted to the southeastern most part of the Appalachian Plateau in West Virginia. It is less than 200 feet thick in Raleigh County and thickens to about 700 feet in McDowell County. It consists primarily of sandstone, with shale and several minable coals (notably the Pocahontas No.3 and 4 seams), and lesser amounts of clay. Figure 2 shows the thickness of cover for the Pocahontas No.3 coalbed.



Isopach Map: Thickness of Cover Over the Pocahontas No. 3 Coalbed (Kelafant et al., 1988)

Figure A6-4

Figure 2. Isopach Map. Thickness of cover over the Pocahontas No.3 Coalbed Pocahontas No. 3 Coal Seam __Avg. Overburden 200-700

The major structural control of drainage is the extensive Elkhorn Creek stress-relief fracture system lineament or photolinear (fracture zone), especially the photolinear that occurs along Elkhorn Creek and adjacent to the residents. (Ferguson, 1967) and
(Wyrick and Borchers, 1981) have demonstrated the model for groundwater flow in the Appalachian Plateau, which results from infiltrating water that descends downslope in a stairstep fashion through stress-relief fractures in the valley walls. It is then interconnected with the horizontal bedding plane fractures in the valley bottoms. Similarly, as a result, the near vertical valley wall fractures are hydrologically connected to horizontal bedding plane fractures that occur in, or that are immediately beneath, the alluvial material in Elkhorn Creek. In some areas the flow system may not be interconnected primarily due to lithostratigraphic control. The Elkhorn Creek streams within the study area are hydrologically connected, in part, due to the shallow groundwater flow regime through the valley stress-relief fracture systems. The extent of stress fracturing and flow are uncertain as no data is available to verify the flow extent.

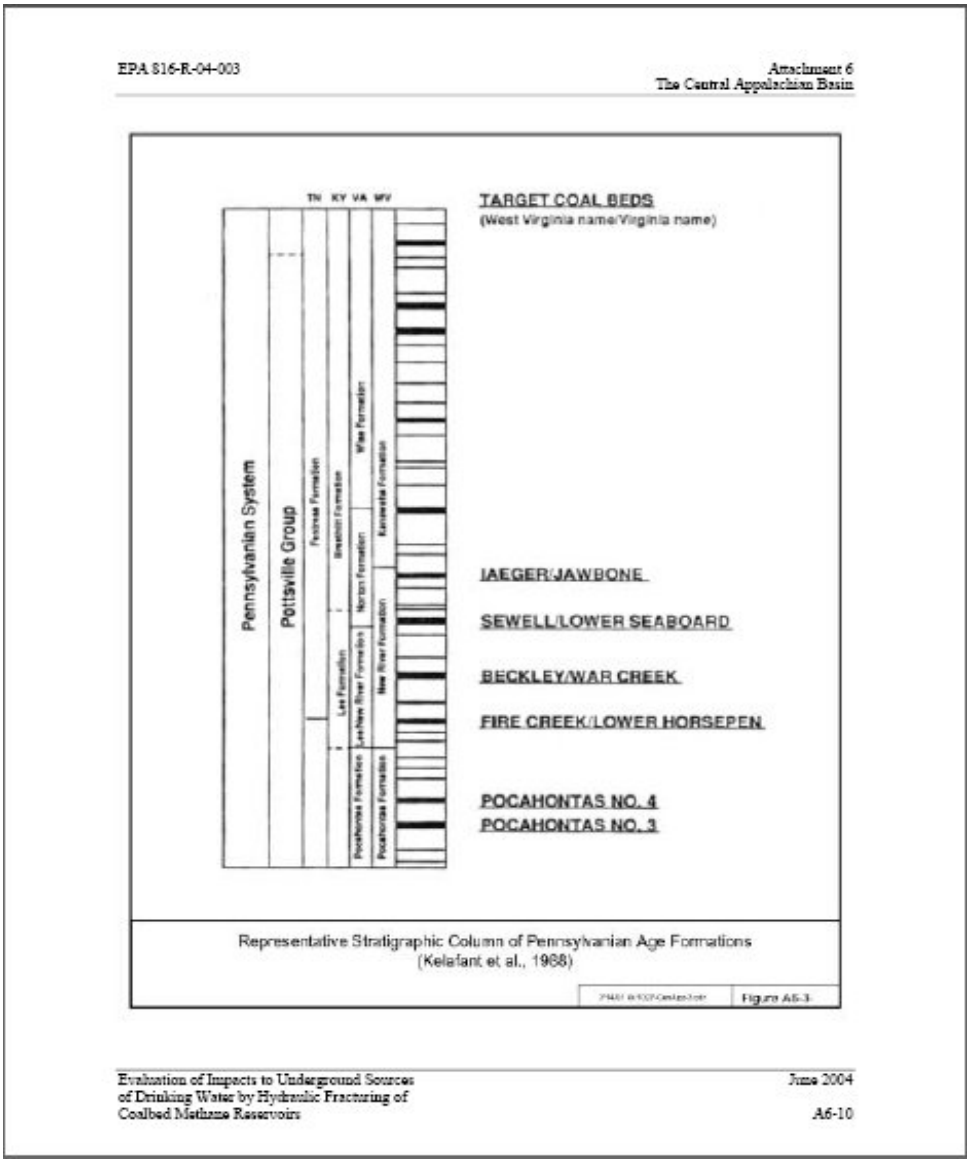


Figure 3. Stratigraphic column of Pennsylvanian Age Formations

HYDROLOGIC BASIN

The primary aquifers in this area are Lower Pennsylvanian aquifers, which include the Pottsville Group (National Water Summary, 1984). Wells are commonly 50 to 300 feet deep and typically produce one to 100 gallons per minute of water (National Water Summary, 1984). The Pocahontas Formation is the main source of groundwater for public consumption in McDowell County. Fractured sandstone is the principal aquifer but shale and coal also yield water to some wells. Underground coal mine voids serve as significant aquifers for public water supply for the McDowell County Public Service District. Aquifer yields usually range from 1 to 50 gal/min from wells 200 feet or less in depth.

Well yields are influenced by well depth, location, and the lithology of the rocks. On average, deeper wells have greater yields; however fractures are generally fewer in number and smaller at greater depths. Wells in the valleys of perennial streams may yield as much as 300 gal/min from wells extended into sandstone of the Pocahontas Formation. Yields from depths greater than 300 feet are probably from intergranular pore space where sandstone particles are poorly cemented (Price and others, 1962).

Groundwater is stored in and moves through intergranular (primary) permeability and fractured (secondary) permeability openings in rocks. The Pocahontas coal seams have been extensively mined for decades in McDowell County creating secondary fracturing in the study area which causes more water to move through fracture openings because they are larger than the intergranular openings. Most of the water from aquifers in this area comes from secondary permeability.

All groundwater is in motion from areas of recharge to areas of discharge. Water moves downward from shallow aquifers to deeper aquifers and laterally to the outcrop of the aquifer. Base flow discharge from the recharge area is shown in (Figure 4).

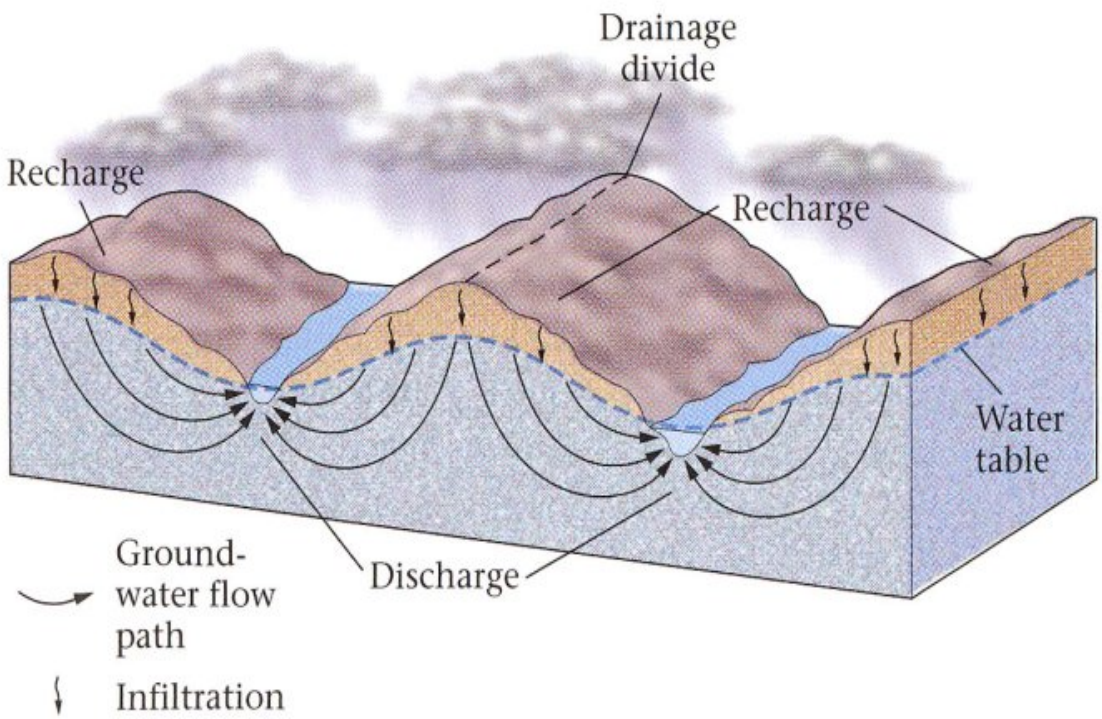


Figure 4. Flow lines from the recharge area top the discharge area curve through the substrate. Some groundwater descends to great depths and then rises back to the surface. (C.W. Fetter, Fourth Edition, Figure 19.9 2001, 1994)

Lateral discharge from an aquifer is seen as seeps or springs on hillsides (Figure 5). The quantity of water recharged to deeper aquifers is controlled by the nature of the underlying rocks and the hydraulic gradient which is shown in (Figure 6). Water in deeper aquifers also can move downward or laterally to become stream flow.

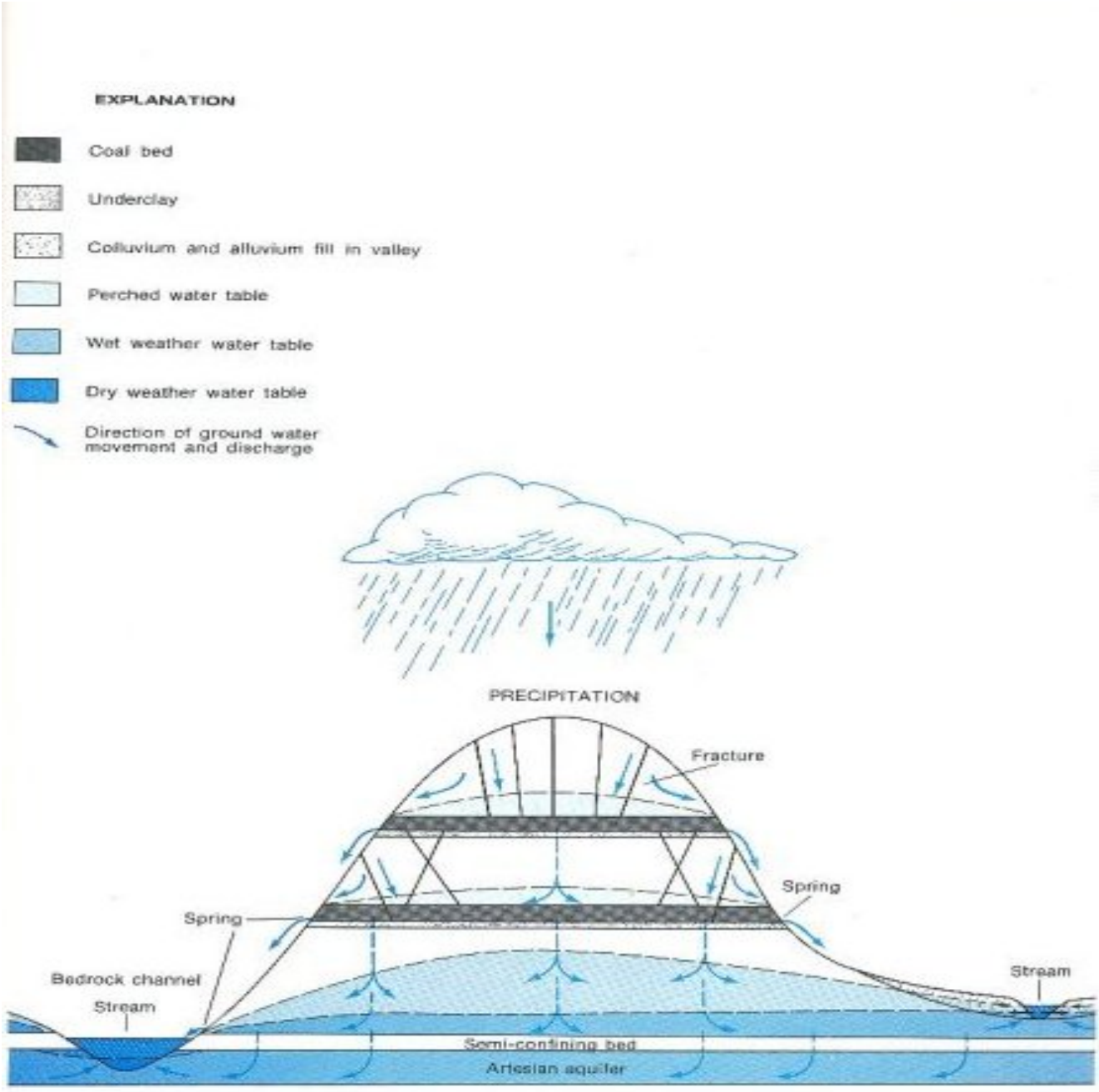


Figure 7.1-1 Generalized water movement in aquifers.

Figure 5. Generalized water movement in aquifers. (USGS)

Anything that moves requires an expenditure of energy and so does groundwater. Hydraulic Head (h) is the energy per unit weight of water h = v2/2g + z + P/y. Groundwater moving from point 1-> 2 Consumes: Hydraulic Head (h) is the energy per unit weight of water h = v2/2g + z + P/y.

Hydraulic gradient is the change in hydraulic head/ distance of flow path dh/dl. Groundwater moves from higher -> lower head

Darcy's Law
Governs the flow through a porous material
Q = -K A dh/dl **(Fetter, 1994)**

Where: K = hydraulic conductivity
A = area
dh/dl = hydraulic gradient

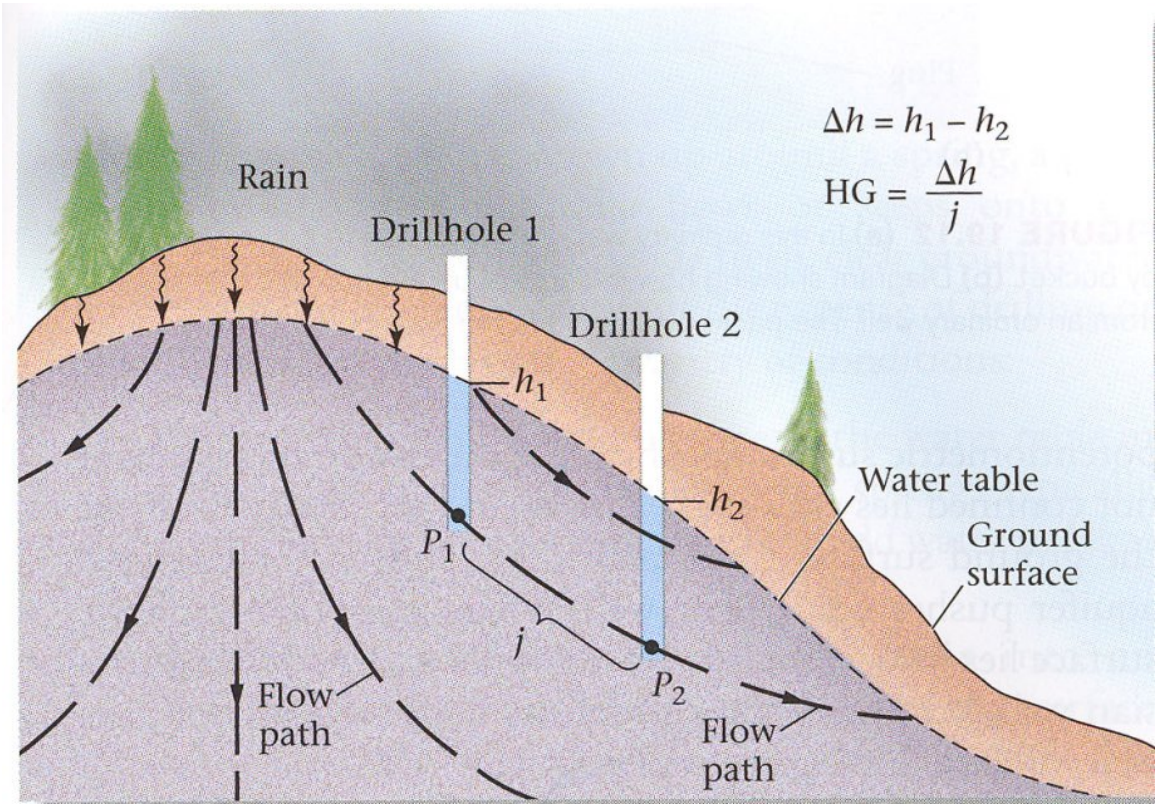


Figure 6. Hydraulic gradient (HG) is the change in hydraulic head per unit of distance between two points (j) along the flow path. (C.W. Fetter. Fourth Edition, Figure 19.11)

DATA REQUIREMENTS FOR THE MODEL

To successfully transform the conceptual model into a mathematical model it was necessary to have a database that provided adequate information to apply the requisite equations. In order to create the groundwater flow model, the physical configuration of the aquifer, including the location, areal extent, and thickness of all the aquifers, and boundary conditions were necessary to define. Important hydraulic properties include the variation of transmissivity or permeability and storage coefficient of the aquifers. Additionally, the variation of permeability and specific storage of the layers and the hydraulic connection between the aquifers and surface-water bodies are equally important to identify.

The conceptual model database coverage's were from GIS coverage for U.S.G.S. Welch 7.5 minute quadrangles (NAD83, Zone 17). The study area within the modeled boundary is approximately 25.6 square miles (See Figure 7) Duplicate layer coverage were created under the boundary coverage theme. The first layer represents the ground surface, second layer representing Pocahontas No.4 coal seam, third layer interburden and fourth layer the Pocahontas No.3 coal seam. Input data for the specified heads were taken from data provided in the UIC permit. A separate coverage was created for the injection well and hydraulic head.

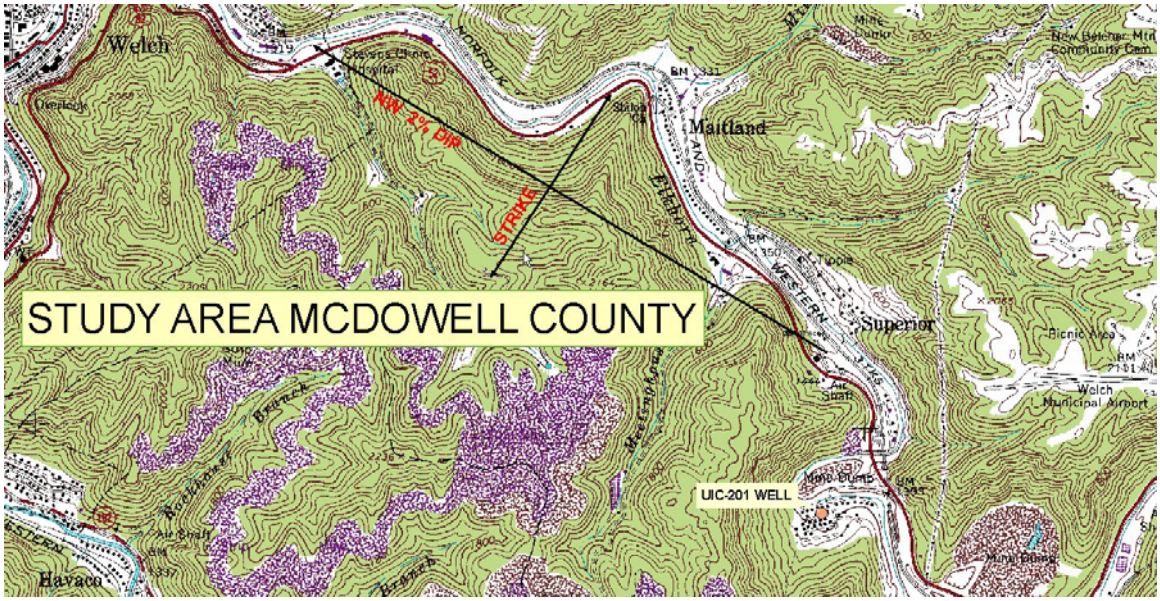


Figure 7. Geographical strike and dip of modeled area.

BOUNDARY CONDITIONS

There are three outside forces acting on groundwater. The most obvious is gravity, which pulls water downward. The second influence is external pressure. Above the zone of saturation, atmospheric pressure is acting. The third force is molecular attraction, which causes water to adhere to solid surfaces.

To solve the groundwater flow equation the boundary conditions were specified. There are two basic types of boundary conditions (Wang & Anderson 1982). If the head is known at the boundary of the flow region it is known as a Dirichlet condition. If the flux across a boundary to the flow region is known it is a Neumann condition. In the area modeled the boundary conditions were mixed, with some portions having known head and some portions having known flux (See Figure 8). The hydraulic boundaries were determined from the topographically high and low areas which are defined as the stream valley of Elkhorn Creek and the mountainous terrain to the west and east.

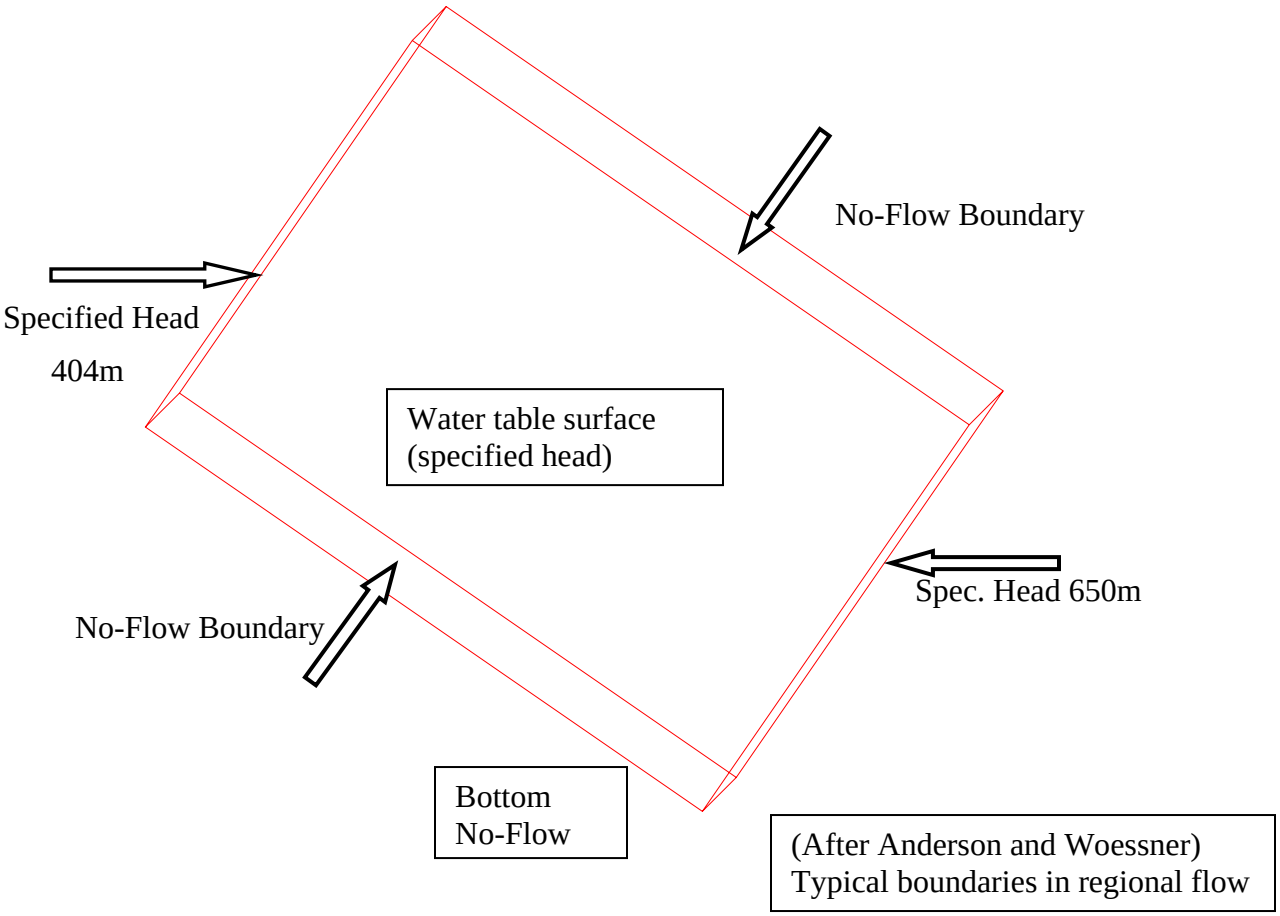


Figure 8.

MODEL DEVELOPMENT USING MODFLOW

The model is three-dimensional in that the previously defined four layers of porous media were stacked with the layers having the same x-y grid dimensions and spacing (See Figure 9). The delta-z dimension is not specified, but is determined indirectly. The transmissivity of each layer (hydraulic conductivity X delta-z) was specified for each layer. The top layer is considered convertible with a top and bottom elevation specified. For each cell the model determines if it is confined (the head is greater than the elevation of the top) or unconfined (the head is less than the elevation of the top). Since the model has multiple layers, a vertical K was determined. This is the harmonic mean of K(z) weighted by delta-z between vertically adjacent cells.(Fetter 1994)

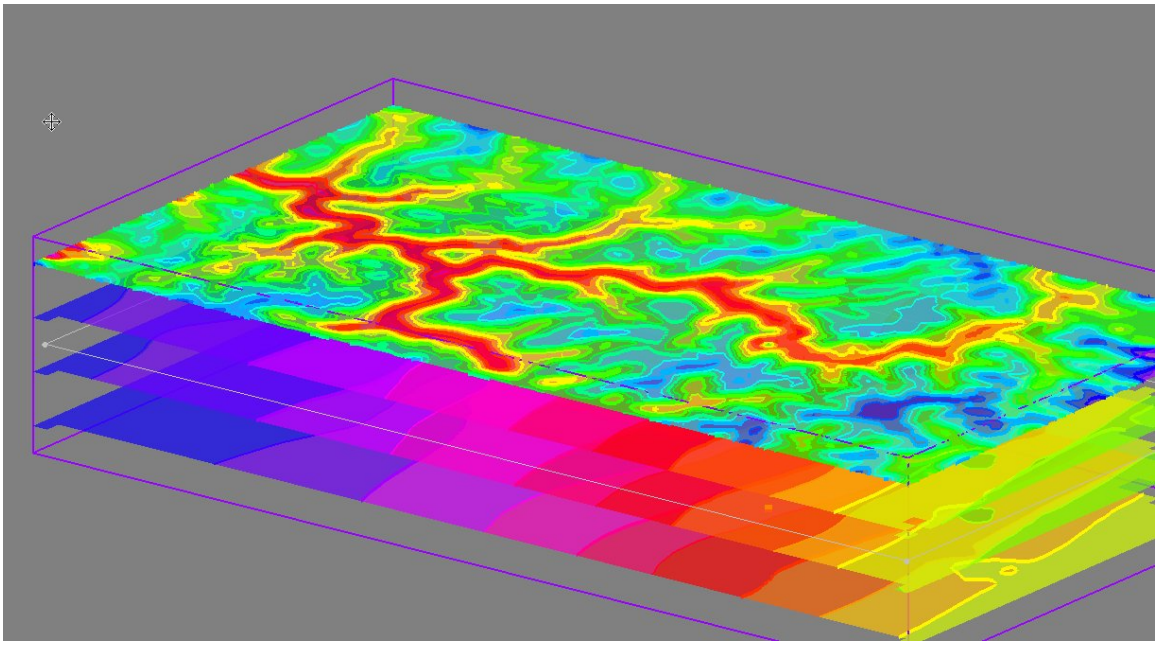


Figure 9. Layers defining model. Colors depict descending hydraulic heads from SE 650m to NW 250m with varying elevations.

Close grid spacing was used in designing the grid in order to capture the steep gradient near the well (See Figure 10). The model will yield the head at the center of the cell. If the cells had been too large, there could have been significant difference in head from one side to the other.

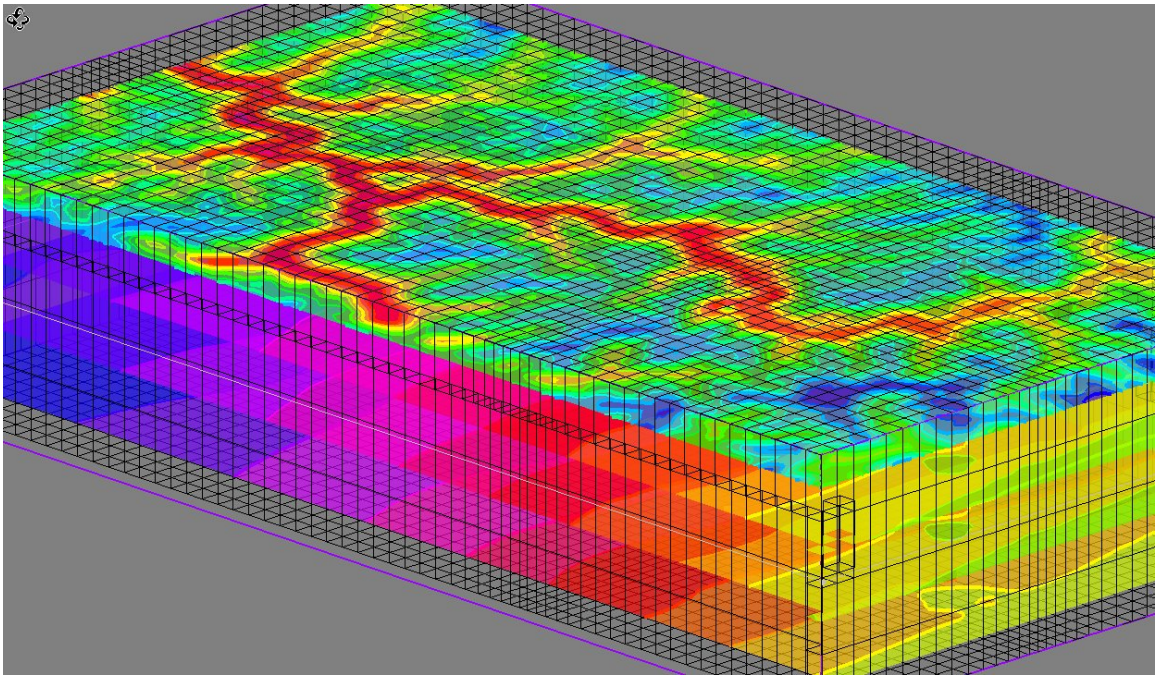


Figure 10. Model grid pattern. A groundwater flow model integrates the laws of groundwater flow with the hydrogeologic framework developed.

The PCG2 (Preconditioned conjugate gradient method) package was used as the solver package. The PCG2 solvers works with the wetting capability. The two most important variables that affected stability in the model were the wetting threshold and identification of which neighboring cells should be wetted. Both of these are controlled through WETDRY. A review of the output file to identify cells that converted repeatedly from wet to dry were most often corrected by raising the wetting threshold for those cells and looking at the boundary conditions associated with dry cells.

The MODPATH package was used for particle tracking. MODPATH is a particle tracking post-processing package that was developed to compute three-dimensional flow paths using output from steady-state or transient groundwater flow simulations by MODFLOW, the U.S. Geological Survey finite-difference groundwater flow model. (David W. Pollock 1994.

MODPATH uses a semi-analytical particle tracking scheme that allows an analytical expression of the particle's flow path to be obtained within each finite-difference grid cell. Particle paths are computed by tracking particles from one cell to the next until the particle reaches a boundary, an internal sink/source, or satisfies some other termination criterion. It appears that from the injection at the well the watertable is erased and a local groundwater high allows some of the flow to traverse in a southeasterly direction before re-establishing a down-dip northwesterly flow path(See Figures 11, 12, and 13).

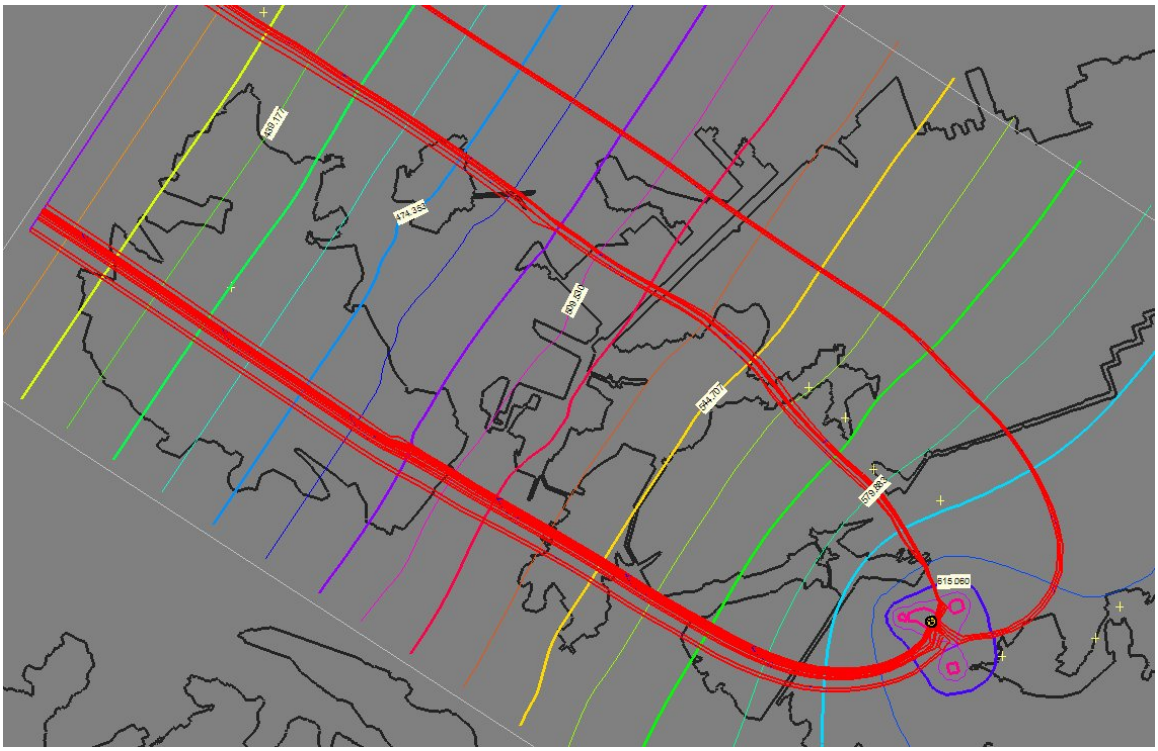


Figure 11. Particle path lines from injection well moving northwest down gradient.

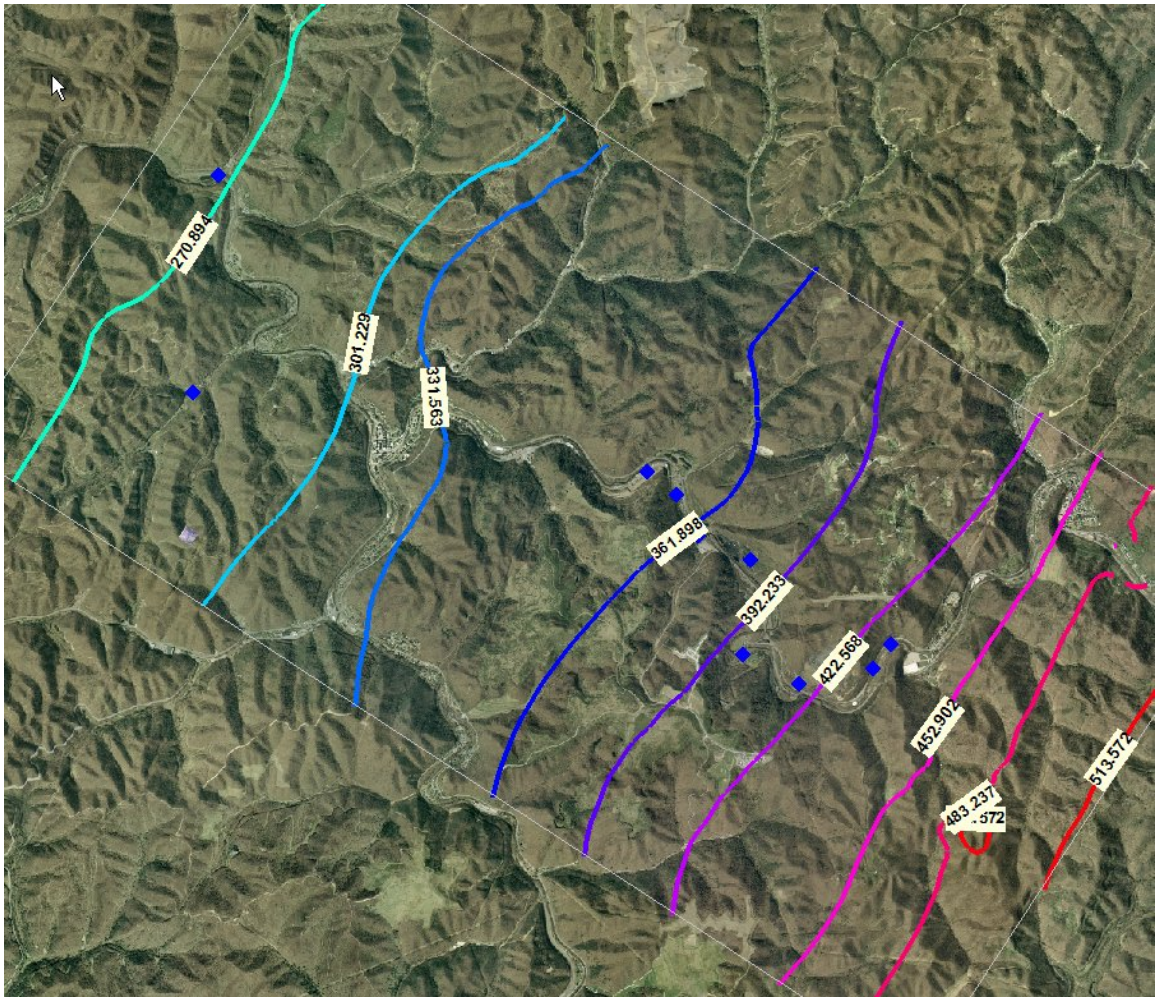


Figure 12. Decreasing hydraulic head in a northwest dip.

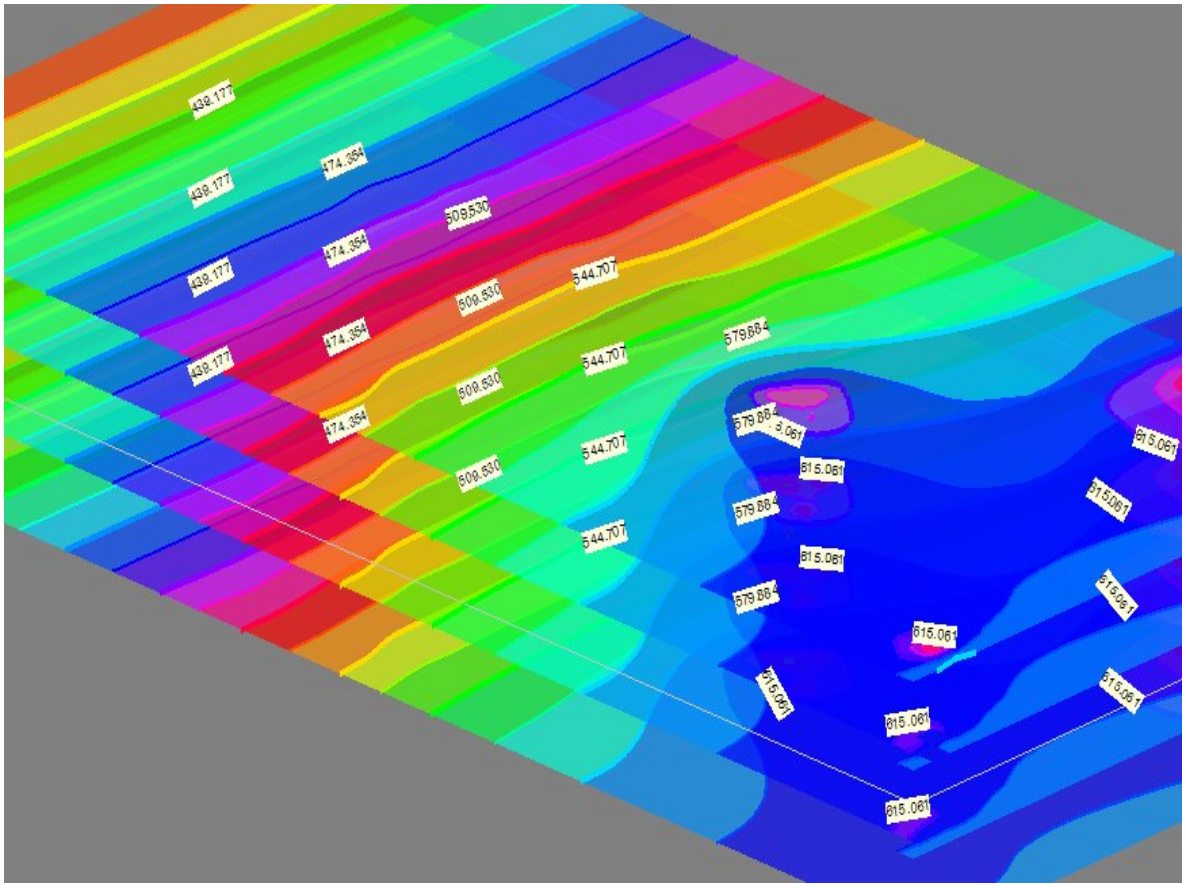
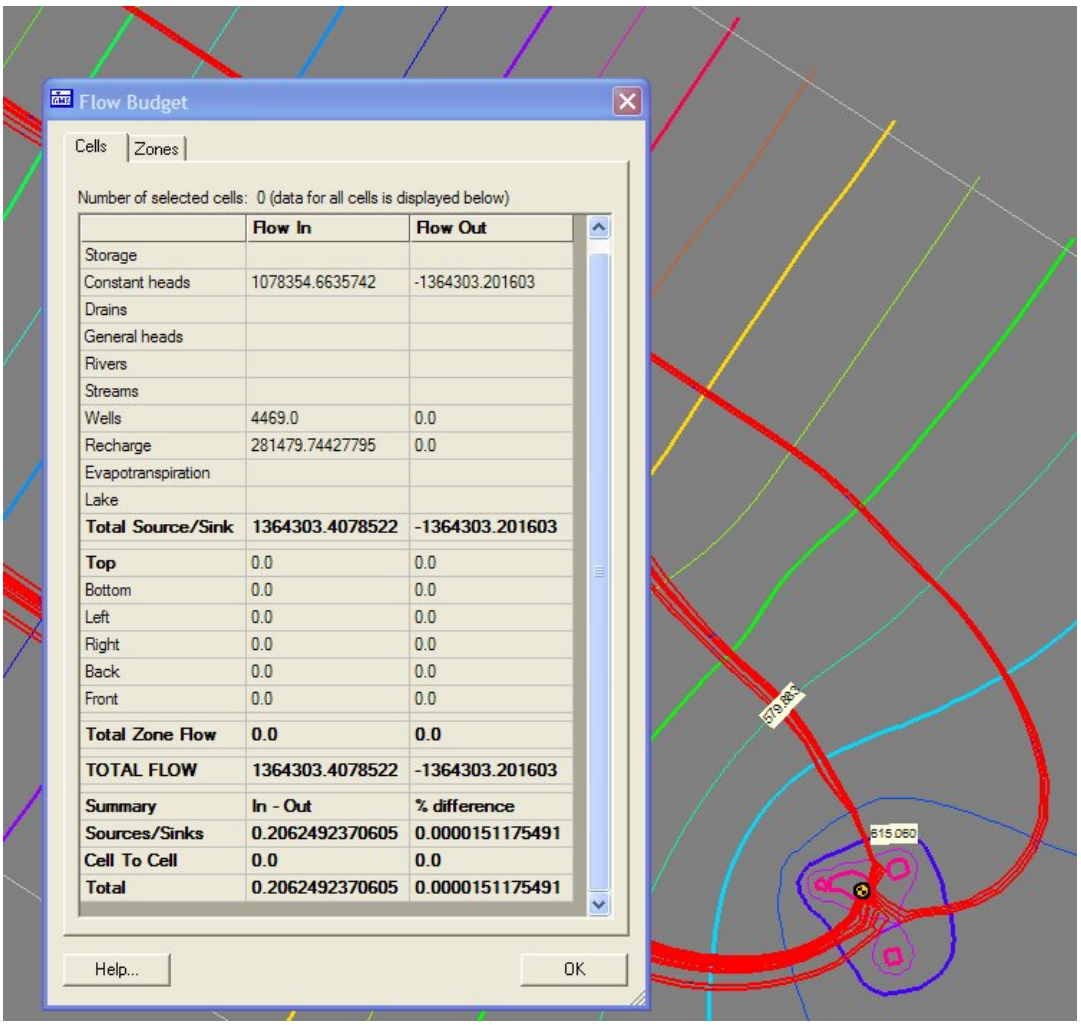


Figure 13. Modeled decreasing hydraulic head values. Colors depict descending hydraulic heads from SE 650m to NW 250m with varying elevations.

Viewing the Flow Budget

Once the zone budget IDs have been assigned, the flow budget for each zone can be viewed by selecting the Flow Budget command in the Data menu that brings up the Flow Budget dialog. There is a new zone selector combo box at the top of the dialog. The flow budget associated with the selected zone is shown in the table. The combo box includes an "All zones" option that displays a summary for all zones in the model. The following table is the computed flow for the model (See Figure 14). The model indicated that 79.04 percent of flow is from the constant head with recharge contributing 20.63 percent to the system and the well only contributing .33 percent.



	Flow In	Flow Out
Storage		
Constant heads	1078354.6635742	-1364303.201603
Drains		
General heads		
Rivers		
Streams		
Wells	4469.0	0.0
Recharge	281479.74427795	0.0
Evapotranspiration		
Lake		
Total Source/Sink	**1364303.4078522**	**-1364303.201603**
Top	0.0	0.0
Bottom	0.0	0.0
Left	0.0	0.0
Right	0.0	0.0
Back	0.0	0.0
Front	0.0	0.0
Total Zone Flow	**0.0**	**0.0**
TOTAL FLOW	**1364303.4078522**	**-1364303.201603**
Summary	**In - Out**	**% difference**
Sources/Sinks	**0.2062492370605**	**0.0000151175491**
Cell To Cell	**0.0**	**0.0**
Total	**0.2062492370605**	**0.0000151175491**

Figure 14. Flow budget summary.

The model closely projected the actual field observations by showing the flooding of cells in areas of discharge or seeps (See Figure 15).

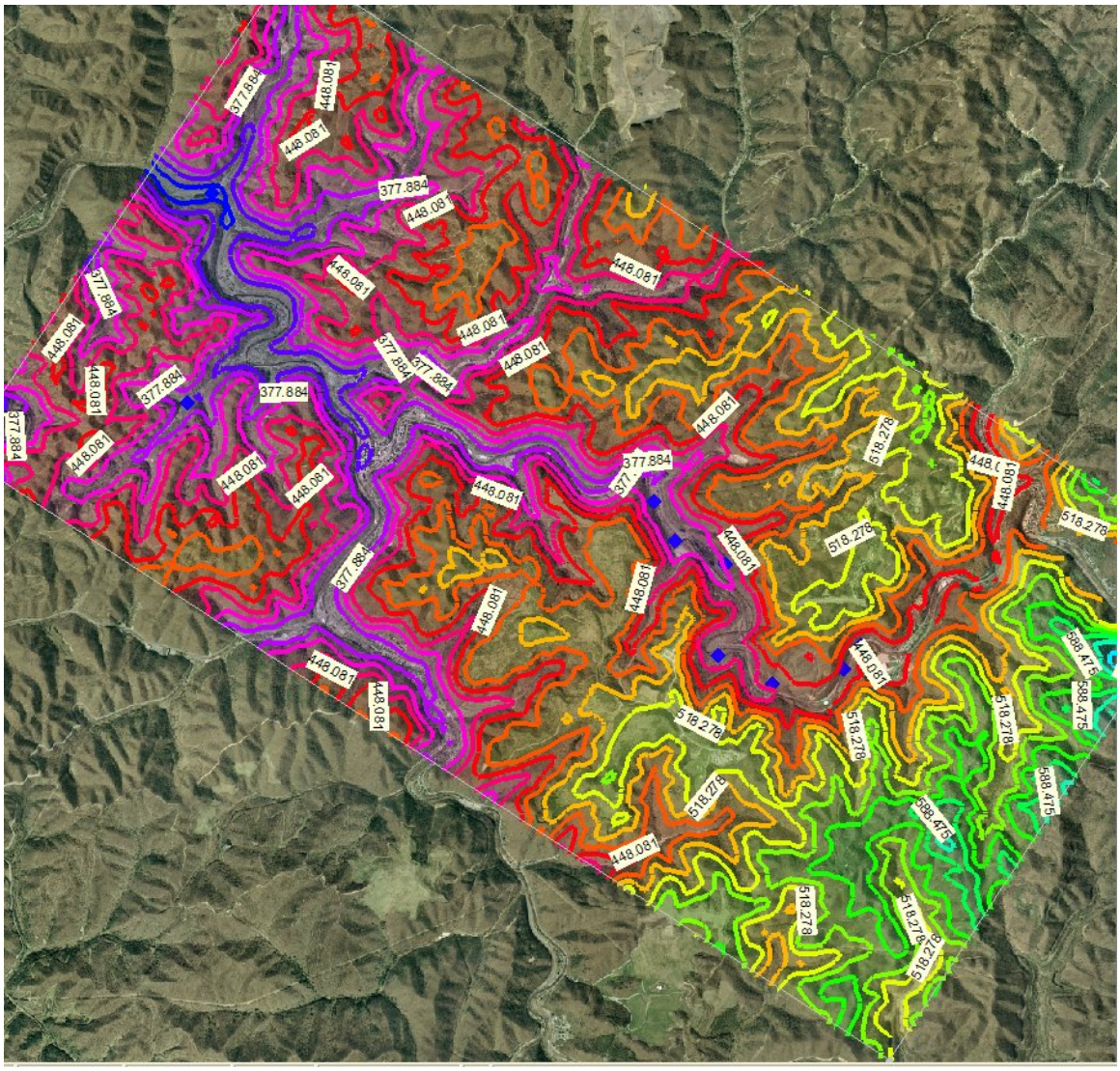


Figure 15. Model projection indicates similarity with field observations.

The flow direction of the MODPATH particle tracking also indicates movement in a northwest down-dip direction. Any potential contaminates from slurry injection would follow this flow path. The study of slurry injection will continue by using MT3DMS module for simulating the migration of contaminant plumes over time.

CONCLUSIONS AND RECOMMENDATIONS

The groundwater model tests how well we understand the actual site conditions by comparing observed and modeled data. Observed and modeled water levels, flow direction, and velocities should be similar.

The following basic assumptions were made about the hydraulic conditions in the aquifer and about the injection well.

1. The aquifer is bounded on the sides and bottom of the model.
2. All geologic formations are horizontal and have infinite horizontal extent.
3. The aquifer is homogeneous and isotropic.
4. All flow is radial toward the well.
5. Groundwater flow is horizontal.
6. Darcy's law is valid.

The modeled area has a northwest dip of approximately 2 percent with a northwest-southeast trend. The conceptual model indicates that flow with decreasing hydraulic head values is in the downgradient direction dipping to the northwest. Figures 13 and 14 illustrate the dip in regard to decreasing hydraulic heads. Since coal contains bedding planes cut by fractures that are called cleats it is assumed that the flow is also following the cleat system as well as mine voids of the coal seams, and flow over the barriers.

The flow direction of MODPATH particle tracking also indicates movement in a northwest down-dip direction. Any potential contaminates from slurry injection would follow the flow path. The study of slurry injection will continue by using MT3DMS module for simulating the migration of contaminant plumes over time.

The model includes assumptions that were necessary for modeling. Many changes could be made in the model to more accurately reflect the true setting.

Continued improvements will be made by:

1. Gathering more data relating to the boundary conditions that apply to the actual aquifer system and the actual flow boundaries that might exist in the area,
2. Expand the boundary on a regional basis to include other major streams,

3. Gather more accurate information relating to the hydraulic conductivity and recharge for the different areas of the model,
4. Precipitation,
5. Evaporation,
6. Transpiration,
7. Runoff, and
8. Sublimation.

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