Application of the Advection-Dispersion Equation in GIS to Analyze the Risks to Groundwater Resources as a Result of Hydraulic Fracturing

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Abstract

This paper describes an approach to hydrogeologic mapping and integrates solutions to fundamental groundwater flow and transport equations that are incorporated within a geographic information system which function on spatial hydrogeologic data. The tools include a discrete form of Darcy's Law to generate flow direction and preserve conservation of mass, a particle tracking procedures to calculate advection along flow paths, and a porous puff dispersion functions to determine distribution of a solute in the porous medium. The model solution allows for calculation of advection and dispersion from a source point along the flow path. The functions are applied in a two-dimensional raster GIS environment. Output features include a flow field, advection path, and a 2-D grid of impacted area of the dispersed constituent. All calculations take place within the native GIS environment. The scope of the research project was to develop a risk assessment model directed towards pollution containment. GIS will be a pivotal technology in current and future analysis to evaluate the risk of drinking water contamination posed by hydraulic fracturing activities.

Introduction

Dunn County, North Dakota is located in West Central North Dakota and has an estimated population of 3500 people. In September, 2010 an oil well (Franchuk 44-20SWH) near Killdeer, North Dakota experienced a uncontrolled blow out during the 5th stage of a 23 stage fracturing operation when the seven inch intermediate casing burst. This resulted in the spilling of approximately 2000 barrels (84,000 gallons) of hydraulic fracturing fluids and oil to the surface (EPA, 2011). At this time it is suspected hydraulic fracturing fluids and oil were released into the subsurface because the surface casing was compromised at 38.5 feet below land surface. During the clean up process approximately 1007 (42,294 gallons) barrels of water and 125 barrels (5250 gallons) of oil were recovered (EPA, 2011). To date it is unknown if groundwater contamination occurred. Ground water is protected during the shale gas fracturing process by a combination of the casing and cement that is installed when the well is drilled (NETL, 2009). Intermediate casing is designed to prevent contamination of the gas that will be produced by freshwater aquifers near the Earth's surface (Zoback, Kitasei, and Coipithorn, 2010). If the borehole is improperly sealed, natural gas, *fracturing* fluids, and formation water containing high concentrations of dissolved solids may be communicated directly along the outside of the wellbore among the target formation, drinking water aquifers, and layers of rock in between (Zoback et al.,

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2010). Contaminants can migrate directly into groundwater from any source that lies within the saturated zone (NETL, 2009). The failure of the cement or casing surrounding the wellbore poses the greatest risk to groundwater resources (All Consulting, 2008). Contaminants may enter the groundwater from the surface by vertical leakage through the seals around hydraulic fracturing well casings, fractures in surface casing, through wells abandoned without proper procedures, or as a result of contaminant disposal of improperly constructed wells (Boulding and Ginn, 2004). Under current federal laws, only surface water discharges are regulated under the Clean Water Act. Furthermore, state laws have not kept pace with the fast development of United States shale which has led to public health concerns. According to the EPA, hydraulic fracturing has potential to impose short-term and long-term impacts on underground and surface drinking water resources (EPA, 2010). Under current U.S. laws, some aspects of shale gas development are regulated by the Clean Water Act, the Clean Air Act, and the Safe Water Drinking Act, but regulation of drilling and hydraulic fracturing occurs at the state levels and varies widely from state to state.

The primary objective of this study was to develop a model scenario in which contamination occurred. Criteria for contamination are based on scenarios of stochastic well blowout, large seepage events from a point source, or leakage from open pit storage ponds as the result of heavy rainfall events. The drilling and hydraulic fracturing of a horizontal shale gas well may typically require 2 to 4 million gallons of water and in many cases fluids may be stored in lined or even unlined open evaporation pits (NETL, 2009). It is worth noting that all 44 horizontal wells within the Murphy Creek HUC-12 have associated open pit storage ponds. The model scenario also tries to account for large rainfall events in which leakage from storage ponds are of concern. The project will utilize a simple advection-dispersion model to determine spatial impacts in the study area. A contamination event based on hydraulic fracturing well Dirkach 34-9H was modeled and the potential impacts on the local watershed were investigated. The scope of the project will concentrate on the effects of advection, dispersion, and particle tracking as they pertain to groundwater movement within the Murphy Creek watershed with the specific aim of risk management.

Natural Gas in the United States

The United States has large quantities of natural gas resources in its domestic shale formations. Horizontal drilling and hydraulic fracturing are the principle technologies that make it possible to harvest methane from its shale source rock.

The Williston Basin is located in the north central United States, underlying much of North Dakota, eastern Montana, northwestern South Dakota, and southern Saskatchewan and Manitoba, Canada. The Bakken Formation exists within the Williston Basin at approximate depths of 11,000 feet at its depocenter, to 4,500 feet deep on the eastern edge of the basin, and up to 3,100 feet deep on the northern edge (EIA, 2006). The Bakken Formation was deposited during the Upper Devonian Period and Lower Mississippian Period, some 417-350 million years ago (American Association of Petroleum Geologists, 1969). Total production of natural gas resources for the United States is estimated at 2,170 trillion cubic feet (Natural Gas Committee, 2011). From

2007-2011, working gas in underground storage for the U.S. lower 48 states has increased by an average of 40.8% (EIA, 2012). The development of shale gas in the U.S. could provide many states with an attractive, lower-carbon domestic fuel while providing jobs and generating significant revenue.

Study Area: Watershed Units

The National Hydrographic Dataset Watershed units in the United States are divided and sub-divided into successively smaller hydrologic units which are classified into four levels: regions, sub-regions, accounting units, and cataloging units (Seaber, Kapinos, and Knapp, 1987). The hydrologic units are arranged within each other from smallest (cataloging units) to largest. Each hydrologic unit is identified by a unique hydrologic unit code (HUC) consisting of two to twelve digits based on the four levels of classification in the hydrologic unit system (Seaber et al., 1987). Cataloging units are also known as HUC-12 and represent individual watershed boundaries. The HUC-12 shapefiles provided by the National Hydrography Dataset were used because features were pre delineated into accurate watersheds.

Methods

Data Sources

The Murphy Creek HUC-12

Murphy Creek HUC-12 was chosen at random for a study area. The Murphy Creek watershed is located in west-central Dunn County and is 30,802 acres (Figure 1). According to the North Dakota Water Commissions (n.d.) well data, the Murphy Creek HUC-12 contains 14 domestic or observational water wells. According to the North Dakota Oil and Gas Division (n.d.), the Murphy Creek HUC-12 contains 44 active, dry, or plugged natural gas wells that could provide a source of contamination (Figure 2). Gas well data were provided by the North Dakota Oil and Gas Division. Downloadable gas and oil well data records are available via ArcIMS server. However, borelog data and geologic information were obtained via a premium subscription service to the North Dakota Oil and Gas Division for $175. Additionally, land surface elevation data was provided by the United States Geologic Survey via a digital elevation model.

Figure 1. HUC-12 Watershed Units in Dunn County, North Dakota.

Groundwater Data

The Killdeer Aquifer is the primary source of drinking water underlying much of Dunn County (EPA, 2011). The aquifer also serves to supply water for drilling operations in the area. The Killdeer Aquifer is classified as a surficial aquifer because it is present above bedrock depth. The area from water level to bedrock depth is known as the saturated zone and determining its thickness was a required variable of the project. Groundwater data were derived from point data obtained from the North Dakota Water Commissions well data. Attributes values utilized for determining groundwater information included elevation, depth to top screen of well, and depth to bedrock. The aquifer was defined by utilizing attribute data for top screen water well depth which is the depth to the top screen of the water well and also used for head elevation values.

Soil Data

Soil data were obtained from the United States Department of Agriculture Natural Resource Conservation Service (USDA-NRCS) (n.d.). The Murphy Creek HUC-12 is comprised of 2088 individual soil sample areas. Within the ArcMap toolbox, the summarize tool was used to generate table data of the most frequent soils in the Murphy Creek HUC-12. The Statistics tool was utilized to isolate the ten most frequent soil types in the watershed (Table 1). The table information was cross referenced against a Soil Legend Report for Dunn County, North Dakota generated from the USDA-NRCS website. The ten soils accounted for a total of 1014 instances out of 2088 total soil occurrences for the Murphy Creek HUC-12 equaling 48.56% of the total soil samples in the Murphy Creek HUC-12. Soil data was used for determining effective porosity when calculating Darcy Flow.

Table 1. Derived from USDA-NRCS Soil Data.

Instances	MUSYM	Unit Name
175	62B	Rhoades silt-loam
132	81C	Vebar-Parshall fine sandy loams
114	52B	Morton-Dogtooth silt loams
101	9D	Sen-Janesburg silt loams
98	81D	Vebar-fine sandy loams
93	52C	Morton-dogtooth silt loams
83	30E	Cohagen-Vebar fine sany loams
79	81B	Vebar-Parshall fine sandy loams
77	106B	Daglum silt loam
62	86F	Brandenburg-Cabba complex

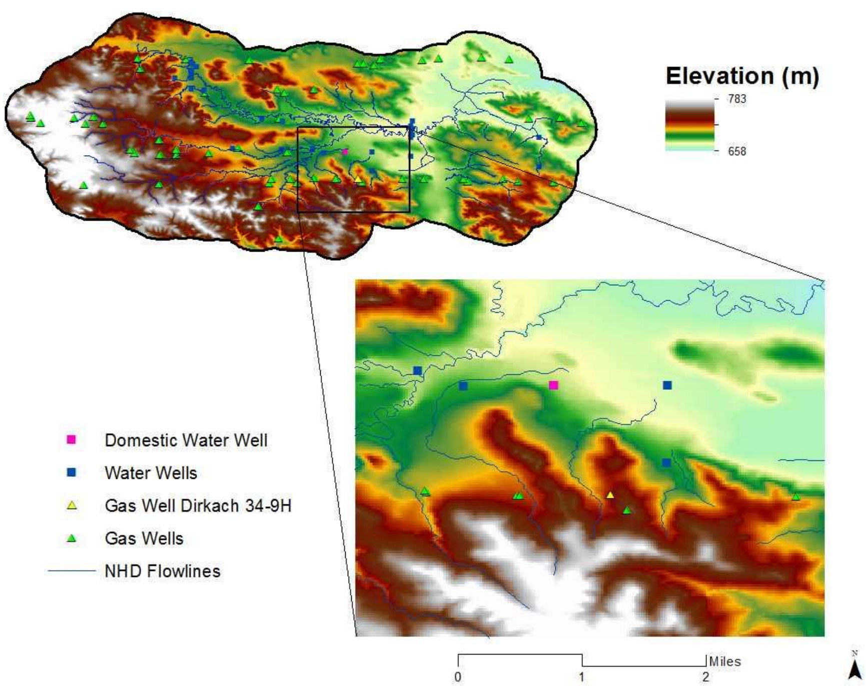

Figure 2. Murphy Creek HUC-12 area of study.

The Advection-Dispersion Model

Generally speaking there are three processes that govern the transport of contaminants in groundwater: advection, dispersion, and retardation. The term advection refers to the movement caused by the flow of groundwater. Advection is calculated based on Darcy's law. In addition, particle tracking can be used to calculate advective transport paths (Walter and Masterson, 2003). Particle tracking is a numerical method by placing a particle into the flow field and numerically integrating the flow path. Additionally, particle tracking can be used to calculate advective paths (Walter and Masterson, 2003). In the model’s behavior, flow is governed by differences between adjacent cells, and calculations were performed through each of the four cell walls independently.

Dispersion in porous material refers to the spreading of a stream or discrete volume of contaminants as it flows through the subsurface (Anderson, 1984). On a macroscopic scale, dispersion is caused by variations in hydraulic conductivity and porosity (NCDENR, 2010). Hydraulic conductivity is a property of the soil and rock that describes how water can move through a porous medium. Effective porosity is the ratio of the voids to the total volume of an unconsolidated or consolidated material (NCDENR, 2010). It is represented by a decimal fraction. Porosity is dependent on the range of grain size and shape of the subject material. Moreover, dispersion is important because it causes the contaminant to spread over a greater volume of aquifer than would be predicted solely from an analysis of groundwater velocity vectors (Anderson, 1984). This spreading effect is of greater concern when hazardous materials are involved. Dispersion is important in predicting transport from point sources of contamination. It is also influential in the spread of non point source contaminants. Additionally, dispersion is important because it may allow contaminants to arrive at a discharge point (e.g., stream or water well) prior to the arrival time calculated from the average groundwater velocity (Anderson, 1984). The accelerated arrival of contaminants at a discharge point is a characteristic feature of dispersion and due to the fact that some parts of the contaminant plume move faster than the average groundwater velocity based on their proximity to the source point, time, and total mass of chemical spill.

The Advection-Dispersion Equation

Most attempts to quantify contaminant transport have relied on a solution of some form of a well-known governing equation referred to as the advection-dispersion equation (Anderson, 1984). Advection refers to the transport of contaminants at the same speed as the average linear velocity of groundwater (V), where:

$$V = \frac{KI}{n}$$

V = velocity of groundwater
K = hydraulic conductivity
I = head gradient
n = effective porosity

The advection-dispersion equation is derived by combining a mass-balance equation with an expression for the gradient of the mass flux (Bear, 1972). Advection is calculated based on Darcy's law (Walter and Masterson, 2003). Darcy’s Law is a generalized relationship for groundwater flow in a porous medium.

It is the fundamental equation for describing flow through porous media. It may be stated in several different forms depending on the flow conditions. Darcy's Law expresses the factors that control groundwater movement as follows:

$$Q = KA\left(\frac{dh}{dl}\right)$$

Q = discharge (volume of water per unit time)
K = hydraulic conductivity
A = cross-section area (at right angle to groundwater flow direction)
dh/dl = head gradient, Δ in head per unit distance

Data Development

Assumptions

The modeling of transport, fate, and impact of solutes in groundwater is a complex problem. The complexity of groundwater flow modeling through porous media can involve dozens of variables to characterize fluid and medium. This research specifically focuses on a simple form of the advection dispersion equation therefore many parameters have been reduced or simplified. The essential elements for modeling flow using Darcy's law require information about the porous medium properties such as hydraulic conductivity, effective porosity, transmissivity, and hydraulic head gradient. Raster datasets are defined continuously over the gridded two-dimensional area of study. Like most computer models, the products developed as a result of this research are mathematically and conceptually ideal and may not accurately simulate natural conditions. The model assumes a steady state. The model shows roughly in which direction transport may be expected and plume of effected area. The equations assume many properties are constant and uniform. The Murphy Creek HUC-12 was chosen at random for a study area in oil and gas producing regions of the Bakken Shale formation. Darcy's Law assumes water is the working fluid. The overall concentration of additives in most slick-water fracturing fluids is relatively consistent 0.5% to 2% with water making up 98% to 99.5% (NETL, 2009). The model scenario was based on an instantaneous release of 1,000,000 gallons or 3785.41 meters^3 of fluid.

Darcy's Law Data Requirements

All rasters require the same geoprocessing environment in terms of extent and cell size. Raster data creation requires all files as floating point rasters. Effective porosity is a property of the underlying soil material and represents the void space within the material that contributes to flow (Tauxe, 1994). The porosity raster was created using the Spatial Analyst toolset. Porosity is assumed to be constant at a rate of 0.4 (Appendix 1). This means that 40 percent of the volume of the porous medium contributes to the fluid flow. Porosity value in this range is typical of the silt sand loamy soils used as sample data. In unconfined aquifers, the head is reflected in the relative elevation of the water table (Nelson, 2002). Head elevation values were obtained via point data from the North Dakota Water Commissions well data. Head elevation values were computed with the Raster Calculator by subtracting top screen water well depth from surface elevation. This produced a 3-D point file that represents relative elevation for the top level of the saturated zone. The same data file can also be used for aquifer head elevation values. Next, the Kriging tool was then used to interpolate the point file into a floating point raster. The Hydrology toolset was utilized in order to identify and fill sinks according to the Darcy Flow methodology outlined by the ESRI Developer Network. Smooth, consistent input rasters with no sources or sinks, such as wells, infiltration, or leakage should produce small residuals, near zero. A zero volume balance residual output raster indicates a balance between flow in and flow out of the cell (ESRI Developer Network, 2012).

In order for the model to have success it must account for transmissivity. Transmissivity is equal to hydraulic conductivity times the aquifer thickness. Aquifer thickness was computed by using water well borehole data and subtracting depth to top screen of the water well (top of saturated zone) from surface elevation. The same process was used for determining the bottom of saturated zone by using depth to bedrock values. The Field Calculator tool was used to subtract the top of saturated zone elevation from the bottom of saturated zone elevation to define points that represents the thickness of the aquifer at each point. The values were later used for an IDW Interpolation to create a raster where each cell value represents the saturated thickness at that location.

The Raster Math tool was used to create the transmissivity raster file. The transmissivity equation used 10^{-5} meters per second as the hydraulic conductivity value representing the sand silt loamy soil medium extracted from Murphy Creek soil data (Appendix 2). Groundwater modeling within ArcGIS is an iterative process. The proper steps must be performed in order for the model to be successful. Darcy Flow, Darcy Velocity, Particle Track and Porous Puff tools were used to solve for flow direction, velocity, and generate a plume of influence. Particle tracking is an algorithm based tool that utilizes a predictor-corrector scheme of calculating the future location of a particle based on the local velocity field as interpolated from the nearest four nearest raster cell centers. The specific track the particle may take in the model system is free floating through the velocity field and independent of location. The Particle Track tool calculates the path of the particulate matter through the velocity field generated by the Darcy Velocity. In addition, groundwater velocity was solved for by using the advection-dispersion equation for the vector line generated by the particle track tool. The calculated values were used as a comparison to values generated from the model.

Results

The Darcy Flow tool created a groundwater balance residual raster with values ranging from 0.121929 to -0.124442. These values indicate that some inconsistencies may have been prevalent in one of the raster datasets. Inconsistencies were likely to have occurred in the form of sinks or depressions in a raster dataset. Residual values however were near zero and thus within the boundary of acceptable values for proper modeling purposes. The tool measured the difference between the flow of water into and out of each cell and the residual raster was used to check the consistency of the groundwater datasets ergo lower residual values near zero indicate a balance of fluid and conservation of mass. Additional Darcy Flow output features included magnitude and direction rasters for use in particle tracking. The Particle Track tool used the output raster features generated from the Darcy Velocity with X,Y coordinates for the source point of pollution. Coordinates for horizontal well Dirkach 34-9H were used as the source point. The product was an ASCII text file of particle tracking data and a vector file of track direction and length. The model generated segments as the track flows through the raster cells. Eight track segments were computed. Each segment corresponded to the distance constituent's traveled as they were subjected to advection through the flow field on a cell by cell basis. Time of advection was preset at twenty four hours and extrapolated by converting decimal values to minutes and hours. The Particle Tracking procedure ran for a total of 30.1 hours. Time and velocity diminished at a sliding scale as distance from point of source increased. Track length was relatively equal with a mean value of 11.98 meters. Overall track length from point source to center of contamination plume was measured at 95.825 meters (Figure 3).

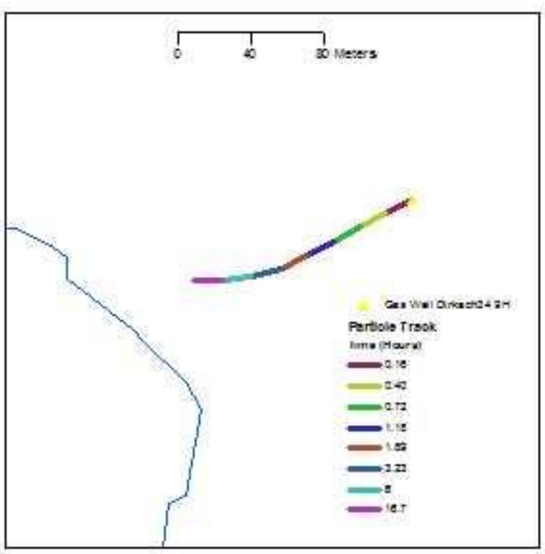

Figure 3. Particle track flow path segments and time (hours) per segment.

Darcy Velocity used Darcy's Law to calculate the flow field which is a vector field of groundwater seepage flow velocities. The Darcy Velocity equation is expressed as:

$$v = \left(\frac{Kdh}{ndl} \right)$$

v = Darcy Velocity
K = 558.135 meters/day
dh = 3.683 meters
dl = 95.825 meters
n = 0.4

Thus, Darcy Velocity calculated from a particle track vector line measuring 95.825 meters with a change in head elevation over that period of 3.683 meters at an instantaneous point source contamination event of 3785.41 $meters^3$ equaled 53.68 meters per day. Comparatively, the computed value equated to 67.1 meters over a 30.1 hour time period. This was compared to the Particle Tracking computed value of 95.825 meters over the same time period. Furthermore, the Darcy Velocity equation was used to calculate groundwater velocity from gas well Dirkach 34-9H to the nearest domestic water well which was located 1500 meters downstream. Groundwater velocity is represented by the following equation where:

$$4.75 m/d = \left(\frac{107.3 * 26.564}{0.4 * 1500} \right)$$

Groundwater transport flowing from the impacted area to the nearest domestic water well in a steady state model can therefore be expected to travel at a rate of 4.75 meters per day.

The Porous Puff tool was used to generate a two-dimensional distribution grid for a solute introduced instantaneously from a specific point into a vertically mixed aquifer. The Porous Puff method worked by calculating the hydrodynamic dispersion of an instantaneous point release of a constituent as it is advected along Particle Track flow path (ESRI, 2012). The tool creates a contamination plume as a result of the specific and instantaneous mass released at the source point. A value of 3,785,411.8 kilograms was used for the point source mass. This value is the kilogram equivalent to 1,000,000 gallons of water used for the spill event. The tool produced a grid of the effect Porous Puff area (Figure 4). A polygon was created from the porous puff grid for determining geometry. The modeled spill event impacted an immediate area of 8.513 acres.

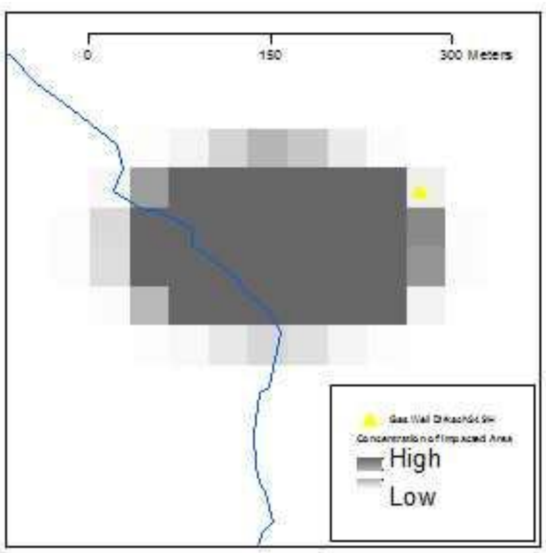

Figure 4. Porous Puff gridded area of contamination. Darker areas indicate greater concentration of contaminates.

Discussion

The model describes a 2-D area of influence in addition to the movement of groundwater contained within the local aquifer. The model shows how advection and dispersive forces may impact an area based on local hydrogeologic factors. Dispersive forces impacted an area of 8.513 acres in the sample area. The data indicated the initial plume of contamination would have an effect on the area watershed. Furthermore, advection forces will cause modeled groundwater velocity to flow at a calculated rate of 53.68 meters per day within the contamination plume. Moreover, advection may transport groundwater at a rate of 4.75 meters per day from the contamination plume towards the nearest domestic well located approximately 1500 meters away. Risk management must differentiate between risks to watershed and risks to groundwater resources; however risk to both would be minimized by decreasing response time as much as possible. This initial contamination plume generated by the Porous Puff tool would be a starting point for risk management response units in an effort to contain toxins and mitigate risks. Furthermore, groundwater velocity values can be used to predict transport of constituents within an aquifer and therefore plays a significant role in a predictive model within the scope of chemical analysis within groundwater. The NHD classifies the down slope drainage in the sample area to be an intermittent stream/river. The USGS defines an intermittent stream/river as one that contains water for only part of the year, but more than just after rainstorms and at snowmelt. Based on this model, negative impact to the local watershed is inevitable; however the level of impact is determinant on many additional variables. Further study would include such variables as dispersivity, retardation factor, and a decay coefficient. The values for decay coefficient would be based each chemical involved in hydraulic fracturing purposes at a well. In addition, toxicity levels for chemicals would need to be determined and chemical samples collected at each segment along the flow path. A full scale chemical analysis combined with a complete advection-dispersion model would give authorities a well calculated assessment of local watersheds and groundwater resources.

Conclusion

The development of shale gas in the United States could provide many states with an attractive low-carbon energy source while providing jobs and generating significant revenue. Domestic shale production of natural gas has the added benefit of lowering the nation's dependency on foreign sources. Opportunity to develop gas resources in the United States cannot be realized unless the environmental risks posed by shale gas development are managed effectively. Addressing the lack of regulatory framework associated with hydraulic fracturing with regard to the application of the Safe Water Drinking Act and the Clean Water Act would make it possible for best practices to be established and disseminated as shale gas continues to expand its prevalence in the United States energy portfolio. Furthermore, a comprehensive analysis of the life-cycle of the relationship between hydraulic fracturing and water resources is necessary to realize the full potential of shale gas in America. Through the use of best practice management, a well-articulated mapping program, and the use of computerized mathematical models it may be possible to mitigate risks posed to drinking water resources by hydraulic fracturing activities in an effort to maximize response to emergency events.

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Appendix 1. Porosity of Geologic Media (Marsily, 1986).

Medium	Total porosity
Unaltered granite and gneiss	0.0002 - 0.018
Quartzite	0.008
Shale, slate, mica schist	0.005 - 0.075
Limestone, primary dolomite	0.005 - 0.125
Secondary dolomite	0.10 - 0.30
Chalk	0.08 - 0.37
Sandstone	0.035 - 0.38
Volcanic tuff	0.30 - 0.40
Sand	0.15 - 0.48
Clay	0.44 - 0.53
Swelling clay, silt	up to 0.90
Tilled arable soil	0.45 - 0.65

Appendix 2. Hydraulic Conductivities of Unconsolidated Media (Marsily, 1986).

Medium	K (m/s)
Coarse gravel	10^{-1} - 10^{-2}
Sand and gravel	10^{-1} - 10^{-5}
Fine sand, silts, loess	10^{-5} - 10^{-9}
Clay, shale, glacial till	10^{-9} - 10^{-13}