Factors Affecting Occurrence and Distribution of Selected Contaminants in Ground Water from Selected Areas in the Piedmont Aquifer System, Eastern United States, 1993-2003

By Bruce D. Lindsey, William F. Falls, Matthew J. Ferrari, Tammy M. Zimmerman, Douglas A. Harned, Eric M. Sadorf, and Melinda J. Chapman

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FOREWORD

The U.S. Geological Survey (USGS) is committed to providing the Nation with credible scientific information that helps to enhance and protect the overall quality of life and that facilitates effective management of water, biological, energy, and mineral resources (http://www.usgs.gov/). Information on the Nation's water resources is critical to ensuring long-term availability of water that is safe for drinking and recreation and is suitable for industry, irrigation, and fish and wildlife. Population growth and increasing demands for water make the availability of that water, now measured in terms of quantity and quality, even more essential to the long-term sustainability of our communities and ecosystems.

The USGS implemented the National Water-Quality Assessment (NAWQA) Program in 1991 to support national, regional, State, and local information needs and decisions related to water-quality management and policy (http://water.usgs.gov/nawqa). The NAWQA Program is designed to answer: What is the condition of our Nation's streams and ground water? How are conditions changing over time? How do natural features and human activities affect the quality of streams and ground water, and where are those effects most pronounced? By combining information on water chemistry, physical characteristics, stream habitat, and aquatic life, the NAWQA Program aims to provide science-based insights for current and emerging water issues and priorities. From 1991-2001, the NAWQA Program completed interdisciplinary assessments and established a baseline understanding of water-quality conditions in 51 of the Nation's river basins and aquifers, referred to as Study Units (http://water.usgs.gov/nawqa/studyu.html).

In the second decade of the Program (2001-2012), a major focus is on regional assessments of water-quality conditions and trends. These regional assessments are based on major river basins and principal aquifers, which encompass larger regions of the country than the Study Units. Regional assessments extend the findings in the Study Units by filling critical gaps in characterizing the quality of surface water and ground water, and by determining status and trends at sites that have been consistently monitored for more than a decade. In addition, the regional assessments continue to build an understanding of how natural features and human activities affect water quality. Many of the regional assessments employ modeling and other scientific tools, developed on the basis of data collected at individual sites, to help extend knowledge of water quality to unmonitored, yet comparable areas within the regions. The models thereby enhance the value of our existing data and our understanding of the hydrologic system. In addition, the models are useful in evaluating various resource-management scenarios and in predicting how our actions, such as reducing or managing nonpoint and point sources of contamination, land conversion, and altering flow and (or) pumping regimes, are likely to affect water conditions within a region.

Other activities planned during the second decade include continuing national syntheses of information on pesticides, volatile organic compounds (VOCs), nutrients, selected trace elements, and aquatic ecology; and continuing national topical studies on the fate of agricultural chemicals, effects of urbanization on stream ecosystems, bioaccumulation of mercury in stream ecosystems, effects of nutrient enrichment on stream ecosystems, and transport of contaminants to public-supply wells.

The USGS aims to disseminate credible, timely, and relevant science information to address practical and effective water-resource management and strategies that protect and restore water quality. We hope this NAWQA publication will provide you with insights and information to meet your needs, and will foster increased citizen awareness and involvement in the protection and restoration of our Nation's waters.

The USGS recognizes that a national assessment by a single program cannot address all water-resource issues of interest. External coordination at all levels is critical for cost-effective management, regulation, and conservation of our Nation's water resources, The NAWQA Program, therefore, depends on advice and information from other agencies—Federal, State, regional, interstate, Tribal, and local—as well as nongovernmental organizations, industry, academia, and other stakeholder groups. Your assistance and suggestions are greatly appreciated.

Robert M. Hirsch
Associate Director for Water

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Conversion Factors and Datum

Multiply	By	To obtain
Length		
inch (in.)	0.0254	meter (m)
foot (ft)	0.3048	meter (m)
mile (mi)	1.609	kilometer (km)
square mile (mi^2)	2.590	square kilometer (km^2)
Flow rate		
cubic foot per second (ft^3/s)	0.02832	cubic meter per second (m^3/s)
gallon per minute (gal/min)	0.06309	liter per second (L/s)
inch per year (in/yr)	25.4	millimeter per year (mm/yr)
Mass		
pound, avoirdupois (lb)	0.4536	kilogram (kg)
Hydraulic conductivity		
foot per day (ft/d)	0.3048	meter per day (m/d)

Temperature in degrees Celsius (°C) may be converted to degrees Fahrenheit (°F) as follows:

$$°F = (1.8 \times °C) + 32$$

Horizontal coordinate information is referenced to the North American Datum of 1983 (NAD 83).

Vertical coordinate information is referenced to the National Geodetic Vertical Datum of 1929 (NGVD 29), unless otherwise noted.

Altitude, as used in this report, refers to distance above the vertical datum.

Specific conductance is given in microsiemens per centimeter at 25 degrees Celsius (µS/cm at 25°C).

Concentrations of chemical constituents in water are given in milligrams per liter (mg/L) or micrograms per liter (µg/L).

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Abstract

Results of ground-water sampling from 255 wells and 19 springs in 11 studies done by the U.S. Geological Survey National Water-Quality Assessment (NAWQA) Program within the Piedmont Aquifer System (PAS) were analyzed to determine the factors affecting occurrence and distribution of selected contaminants. The contaminants, which were selected on the basis of potential human-health effects, included nitrate, pesticides, volatile organic compounds (VOCs), and radon.

The PAS was subdivided on the basis of the general rock type of the aquifers into three areas for the study—crystalline, carbonate, and siliciclastic. The 11 studies were designed to areally represent an individual aquifer rock type and overall are representative of the PAS in their distribution; 7 studies are in the crystalline-rock aquifers, 3 studies are in the siliciclastic-rock aquifers, and 1 study is in the carbonate-rock aquifers. Four of the studies were focused on land use, 1 in an agricultural area and 3 in urban areas. The remaining studies had wells representing a range of land-use types.

Analysis of results of nitrate sampling indicated that in 8 of the 10 areas where nitrate concentrations were measured, median concentrations of nitrate were below 3 mg/L (milligrams per liter); 2 of the 10 areas had statistically significant higher median concentrations when compared to the other 8 areas. The agricultural land-use study in the carbonate-rock aquifer in the Lower Susquehanna River Basin had the highest median nitrate concentration (11 mg/L), and 60 percent of the wells sampled exceeded the U.S. Environmental Protection Agency (USEPA) Maximum Contaminant Level (MCL) of 10 mg/L. The major aquifer study in the crystalline-rock aquifer of the Lower Susquehanna River Basin Study Unit had the second-highest median nitrate concentration. Nitrate concentrations were positively correlated to the percentage of agricultural land use around the well, the total input of nitrogen from all sources, dissolved oxygen concentration, lithology, depth to water, and soil-matrix characteristics. A linear regression model was used to determine that increases in the percentage of agricultural land use, the input of nitrogen from all sources, and dissolved oxygen were the most significant variables affecting increased concentration of nitrate. A logistic regression model was used to determine that those same factors were the most significant variables affecting whether or not the nitrate concentration would exceed 4 mg/L.

Of the analysis of samples from 253 wells and 19 springs for 47 pesticides, no sample had a pesticide concentration that exceeded any USEPA MCL. The most frequently detected pesticide was desethyl atrazine, a degradation product of atrazine; the detection frequency was 47 percent. Other frequently detected pesticides included atrazine, metolachlor, simazine, alachlor, prometon, and dieldrin. Detection frequency was affected by the analytical reporting limits; the frequency of detection was somewhat lower when all pesticides were censored to the highest common detection limit. Source factors such as agricultural land use (for agricultural herbicides), urban land use (for insecticides), and the application rate were found to have positive statistical correlations with pesticide concentration. Transport factors such as depth to water and percentage of well-drained soils, sand, or silt typically were positively correlated with higher pesticide concentrations.

Sampling for VOCs was conducted in 187 wells and 19 springs that were sampled for 59 VOCs. There were 137 detections of VOCs above the common censoring limit of 0.2 µg/L. The most frequently detected VOCs were chloroform, a trihalomethane, and methyl-tert butyl ether (MTBE), a fuel oxygenate. Seventy-nine wells had at least one VOC detected. The detections were related to land use and well depth. Kendall's tau correlations indicated a significant positive correlation between chloroform concentration and urban land use, leaking underground storage tanks, population density, and well depth. MTBE concentrations also were positively correlated to urban land use, leaking underground storage tanks, population density, and well depth.

Radon was sampled at 205 sites. The subdivisions used for analysis of other contaminants were not adequate for analysis of radon because radon varies on the basis of variations in mineralogy that are not reflected by the general lithologic categories used for the rest of the studies. Concentrations of radon were highest in areas where the crystalline-rock aquifers had felsic mineralogy, and the lowest concentrations of radon were in areas where the crystalline-rocks aquifer had mafic mineralogy. Water from wells in siliciclastic-rock aquifers had concentrations of radon lower than that in the felsic crystalline-rock aqui-

fers. More than 90 percent of the wells sampled for radon exceeded the proposed MCL of 300 pCi/L (picoCuries per liter); however, only 13 percent of those wells had concentrations in water that exceeded the alternative maximum contaminant level (AMCL), a higher level that can be used by municipalities addressing other sources of radon exposure.

Overall, concentrations of constituents were related to land-use factors for nitrate, pesticides, VOCs, and to aquifer lithology for radon. None of the 47 pesticides or 59 VOCs analyzed exceeded the MCLs where those constituents were sampled. Concentrations exceeded the MCL for nitrate in 11 percent of the wells sampled. Nearly 91 percent of the wells sampled exceeded the proposed MCL for radon. Additional sampling in selected areas would improve overall understanding of the PAS and increase the possibility of creating predictive models of ground-water quality in this area.

Introduction

The National Water-Quality Assessment (NAWQA) Program of the U.S. Geological Survey (USGS) has conducted studies of ground-water quality throughout large parts of the United States, typically in major river basins, which are termed study units (fig. 1). During the first decade of the program (1991-2000, referred to as Cycle I), most of the analysis and reporting of ground-water quality were done at the level of the study unit. Results for selected contaminants were synthesized on a national level. In the second decade of the program (2001-2010, referred to as Cycle II), the emphasis is on regional reporting of ground-water quality, and results are being compiled for several of the major aquifers. This report is a compilation and analysis of the data from all of Cycle I and the first 3 years of Cycle II for the Piedmont Aquifer System (PAS) of the eastern United States.

Purpose and Scope

This report describes factors affecting the occurrence and distribution of nitrate, selected pesticides, selected volatile organic compounds (VOCs), and radon in ground water from NAWQA studies conducted from 1993 through 2003 in the PAS of the eastern United States. These contaminants were selected for study on the basis of potential for human-health effects. Ground-water samples from 255 wells and 19 springs sampled in 11 studies from selected areas in the USGS NAWQA Program form the basis of this study. These studies include six major-aquifer studies, four land-use studies, and one drinking-water supply study. This report also includes descriptions of the Piedmont bedrock aquifers, the NAWQA ground-water study areas, the NAWQA well networks, and statistical methods used to analyze the water-quality data.

Description of Study Area

The PAS covers an area of about 93,000 mi^2 (fig. 1). The boundaries of the PAS are considered to be coincident with the boundary of the Piedmont Physiographic Province. The Piedmont is bounded on the south and east by the Fall Line and the Coastal Plain Physiographic Province and on the north and west by the Blue Ridge, Valley and Ridge, and the New England Physiographic Provinces (Fenneman and Johnson, 1946). The Piedmont is a transitional area between the unconsolidated sedimentary deposits in the Coastal Plain and the more mountainous regions inland and generally is characterized by low, rolling hills. The Piedmont extends almost 1,000 mi from the southern part of New York State in the north to eastern Alabama in the south and has a maximum width of about 125 mi (Hunt, 1967) (fig. 1).

The PAS includes parts of nine NAWQA study units. The following is a list of the study units, standard study-unit abbreviations, and citations of reports summarizing findings within each area: Long Island and New Jersey Coastal Drainages (LINJ; Ayers and others, 2000), Delaware River Basin (DELR; Fischer and others, 2004), Lower Susquehanna River Basin (LSUS; Lindsey and others, 1998), Potomac River Basin and Delmarva Peninsula (PODL; Ator and others, 1998; Denver and others, 2004), Albemarle-Pamlico Drainages (ALBE; Spruill and others, 1998), Santee Basin and Coastal Drainages (SANT; Hughes and others, 2000), Georgia-Florida Coastal Plain (GAFL; Berndt and others, 1998), Appalachicola-Chattahoochee-Flint River Basins (ACFB; Frick and others, 1998), and Mobile River and Tributaries (MOBL; Atkins and others, 2004) (fig. 1). The Potomac River Basin and Delmarva Peninsula (PODL) study unit is a Cycle II study that combined the Cycle I Potomac River Basin (POTO) and the Delmarva Peninsula (DLMV) pilot studies; however, only the POTO study unit included any part of the PAS. Discussions of Cycle I activities will refer to the POTO study unit and discussions of Cycle II activities will refer to the PODL study unit. NAWQA studies are based on surface drainage basins; however, only selected parts of each study unit are covered by ground-water studies. Of the nine study units that include part of the Piedmont, only six of these included the PAS in their ground-water studies. Additionally, only one of the NAWQA study units sampled the entire area where the PAS intersected their study unit, the other five sampled a subset of the PAS in their study unit. Therefore, the areas where NAWQA study units overlap the PAS (fig. 1) does not represent the areas where NAWQA ground-water studies were conducted.

Physiography and Geology

The PAS is divided into two physiographic sections (Fenneman and Johnson, 1946). These sections generally correspond to the basic rock types found in the PAS. The largest physiographic section in the PAS is the Piedmont Upland Physiographic Section, which is generally the area shown as the

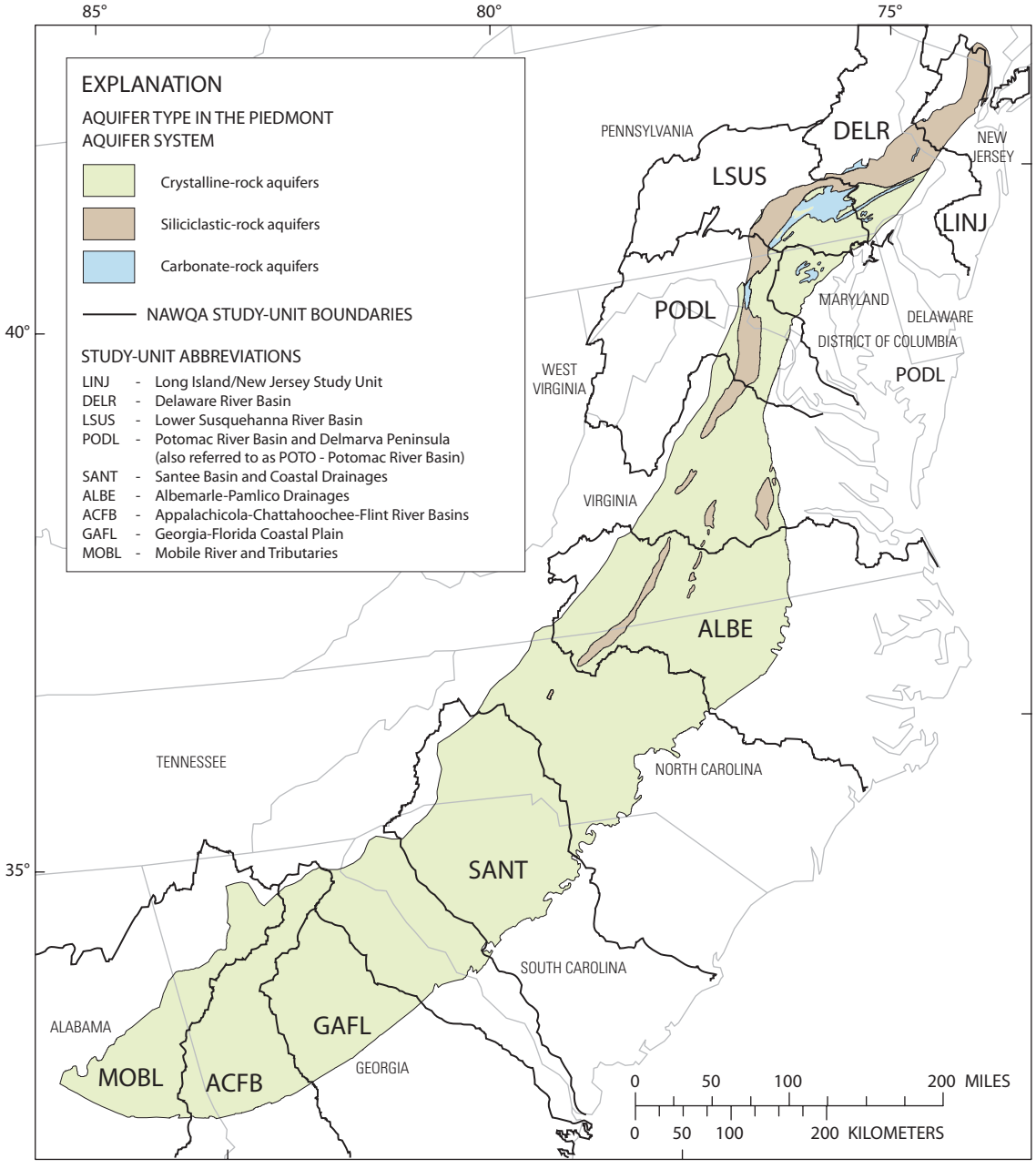

Figure 1. Location of National Water-Quality Assessment Study Units and the aquifer types within the Piedmont Aquifer System, eastern United States (Miller, 1990; Trapp and Horn, 1997).

crystalline-rock aquifers on figure 1. The rocks in the Piedmont Upland are primarily igneous and metamorphic rocks, hereafter called crystalline rocks, that are resistant to erosion and form hilly terrain. The aquifers in the area underlain by crystalline rocks are referred to as the crystalline-rock aquifers (fig. 1). The Piedmont Lowlands Physiographic Section is made up of siliciclastic rocks or carbonate rocks. The area shown as the carbonate-rock aquifers in Pennsylvania and Maryland (fig. 1) is part of the Piedmont Lowlands Physiographic Section. The bedrock in this area is limestone, dolomite, or marble of Paleozoic age; the aquifers in the area underlain by carbonate bedrock are referred to as the carbonate-rock aquifers (fig. 1). The area shown as the siliciclastic-bedrock aquifers (fig. 1) is also part of the Piedmont Lowlands Physiographic Section. In some states, more specific names are given to the siliciclastic part of this physiographic section, such as the Gettysburg-Newark Lowlands in Pennsylvania (Sevon, 2000). The siliciclastic rocks can be locally intruded by diabase; however, only the areas underlain by siliciclastic rocks are included in this study. The aquifers in the area underlain by siliciclastic bedrock are called the Early Mesozoic Aquifers in the U.S. Geological Survey (USGS) Ground Water Atlas (Trapp and Horn, 1997); however, for purposes of this report, these aquifers are referred to as siliciclastic-rock aquifers so that each aquifer is named according to the underlying bedrock rather than the age (fig. 1). Because the siliciclastic aquifers are within the Piedmont Physiographic Province, they are included as a part of the Piedmont Aquifer System. These three basic rock types (crystalline, siliciclastic, and carbonate) form the three basic units used to subdivide the PAS. The crystalline-rock aquifers make up 92 percent of the land within the Piedmont Physiographic Province (fig. 1). Siliciclastic- and carbonate-rock aquifers are 7 and 1 percent of the Piedmont Physiographic Province, respectively.

Land Use and Population and Water Use

The predominant land use in the PAS is forested land; forests cover about 66 percent of the area. Agricultural land covers about 23 percent of the area, and urban land is about 6 percent of the area (Vogelmann and others, 1998a, 1998b) (table 1). The distribution of these land uses in the PAS is highly variable. The land-use variation within the PAS has a trend from north to south; more urban and agricultural lands are in the northern part of the Piedmont. Land use in Piedmont studies from Virginia north had more than 60 percent agricultural and urban land use. More forested areas are in the southern part of the Piedmont; land use in the studies in the Piedmont south of Virginia had more than 60 percent forested land use (Vogelmann and others, 1998a, 1998b) (fig. 2). The most dense urban areas are in the LINJ study unit, the DELR study unit, and the eastern part of the POTO study unit. These areas are underlain by the siliciclastic-rock aquifer, which has one of the highest percentages of urban land (15 percent). The carbonate-rock aquifer also has 15 percent of its area covered by urban land; however, it also has the most dense agricultural activity (63 percent). The crystalline-rock aquifer has the largest proportion of forested land (68 percent). Land use is discussed in greater detail with regard to the land-use distribution within each study unit.

Table 1. Percentage of land use by major subdivisions of Piedmont Aquifer System.

Land-use category[1]	Aquifer			
	Piedmont aquifer system	Carbonate-rock aquifers	Siliciclastic-rock aquifers	Crystalline-rock aquifers
	Land use, in percent of total area			
Urban[2]	6	15	15	5
Forested[3]	66	18	42	68
Agricultural[4]	23	63	37	22
Other	5	4	6	5

[1]Vogelman and others (1998a, 1998b).

[2]Category includes low-intensity residential, high-intensity residential, and commercial/industrial/transportation.

[3]Category includes deciduous forest, evergreen forest, and mixed forest.

[4]Category includes hay/pasture and row crop.

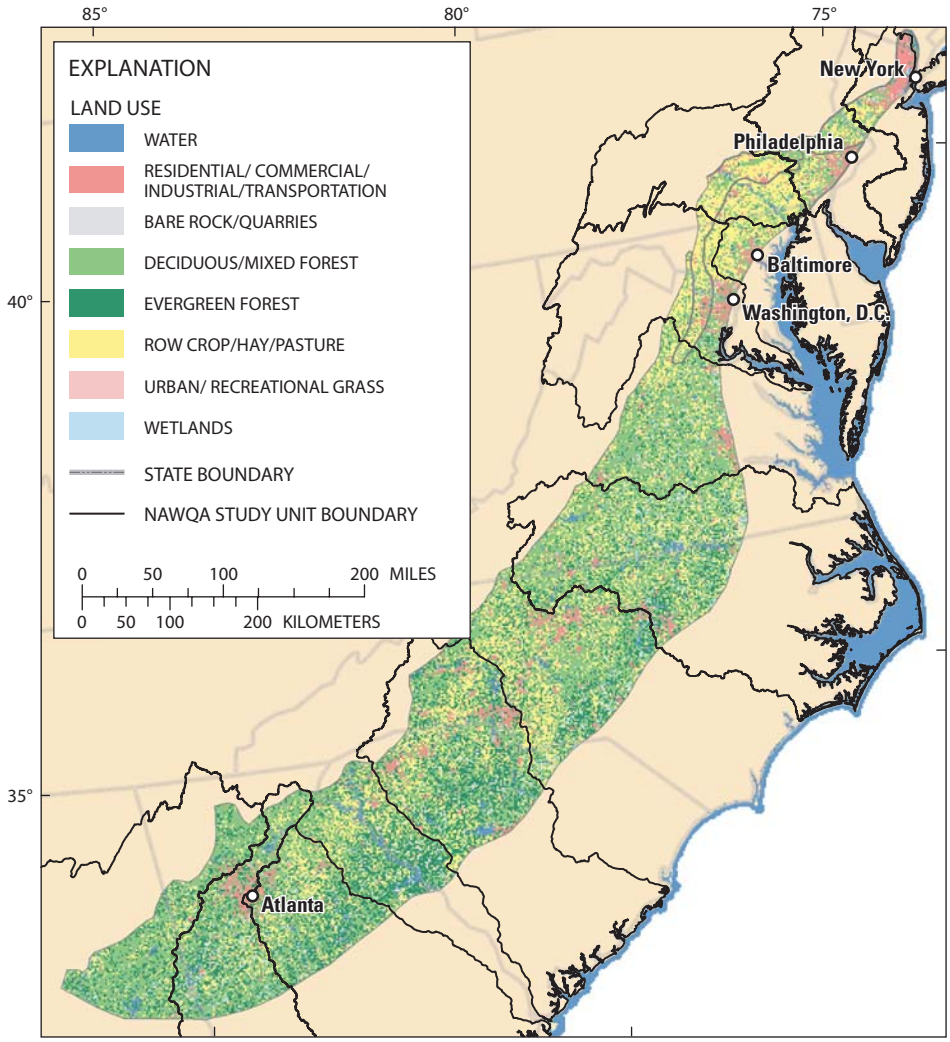

Figure 2. Land use in the Piedmont Aquifer System, eastern United States (land-use data from Vogelmann and others, 1998a, 1998b).

The population of the area underlain by the crystalline-rock aquifers is approximately 16 million (Solley and others, 1998) (all population and water-use statistics cited are prorated based on percentage of county within the study area for border counties). Population and land use are closely related. The population density follows an expected pattern, with the most densely populated areas being in the vicinity of New York, Philadelphia, Baltimore, Washington, D.C., and Atlanta (fig. 2). These cities are not all entirely within the Piedmont; however, the rapidly growing counties around these cities are in the Piedmont. The population of the area underlain by the carbonate-rock aquifers is approximately 500,000. Population density is greater than in the crystalline-rock aquifer area, with about 500 persons per square mile. The population of the area underlain by the siliciclastic-rock aquifers is approximately 5.5 million. The most densely populated parts of the siliciclastic-rock aquifers are central New Jersey, southeastern Pennsylvania, Maryland, and northern Virginia (fig. 2).

Water used for public supply is primarily from surface water in the crystalline-rock aquifers, with only about 1 million residents (6 percent) relying on ground water for public supply. An additional 3.7 million (22 percent) rely on ground water for domestic self-supply (Solley and others, 1998). Overall, about 4.7 million people, or 28 percent of the population, rely on ground water in the crystalline-rock aquifers. The total withdrawals from the crystalline-rock aquifers are approximately 451 million gallons per day. Water use for public supply is primarily from surface water in carbonate-rock aquifer, with about 57,000 (12 percent) relying on ground water for public supply. An additional 155,000 (32 percent) rely on ground water for domestic self-supply. Overall, about 212,000 people, or 44 percent of the population, rely on ground water in the carbonate-rock aquifer. Withdrawals of ground water from the carbonate-rock aquifers total 24 million gallons per day. Ground-water use from siliciclastic-rock aquifers for public supply is more significant than that of the other two aquifers, with about 1.1 million (21 percent) relying on ground water for public supply. An additional 723,000 (13 percent) rely on ground water for domestic self-supply. Overall, nearly 2 million people, or 35 percent of the population, rely on the siliciclastic-rock aquifer. Withdrawals of ground water from the siliciclastic-rock aquifer total 218 million gallons per day. Ground-water pump-

ing rates are highest in the siliciclastic-rock aquifers, with about seven times greater withdrawal rate in million gallons per day per square mile than the crystalline-rock aquifers.

Climate

Characteristics of ground-water flow are affected by climate in several ways. One way is that long-term climate affects the weathering of bedrock, which in turn alters the storage and flow of ground water in the rock. The weathering of bedrock also alters the characteristics of the overburden above the bedrock. Another way that climate affects ground-water flow is that precipitation is a driving force in the ground-water-flow system; therefore, variations in precipitation (and subsequently, recharge) have a large effect on ground-water flow.

Temperature

Average annual temperatures vary from north to south in the PAS (Falcone, 2004). The coldest average annual temperature is 10°C in Pennsylvania and New Jersey, and the warmest average annual temperature is 18°C in South Carolina, Georgia, and Alabama (fig. 3). The average temperature in January is -3.0°C in Pennsylvania and 8.3°C in Georgia. The average temperature in July is 21.7°C in Pennsylvania and 26.7°C in Georgia.

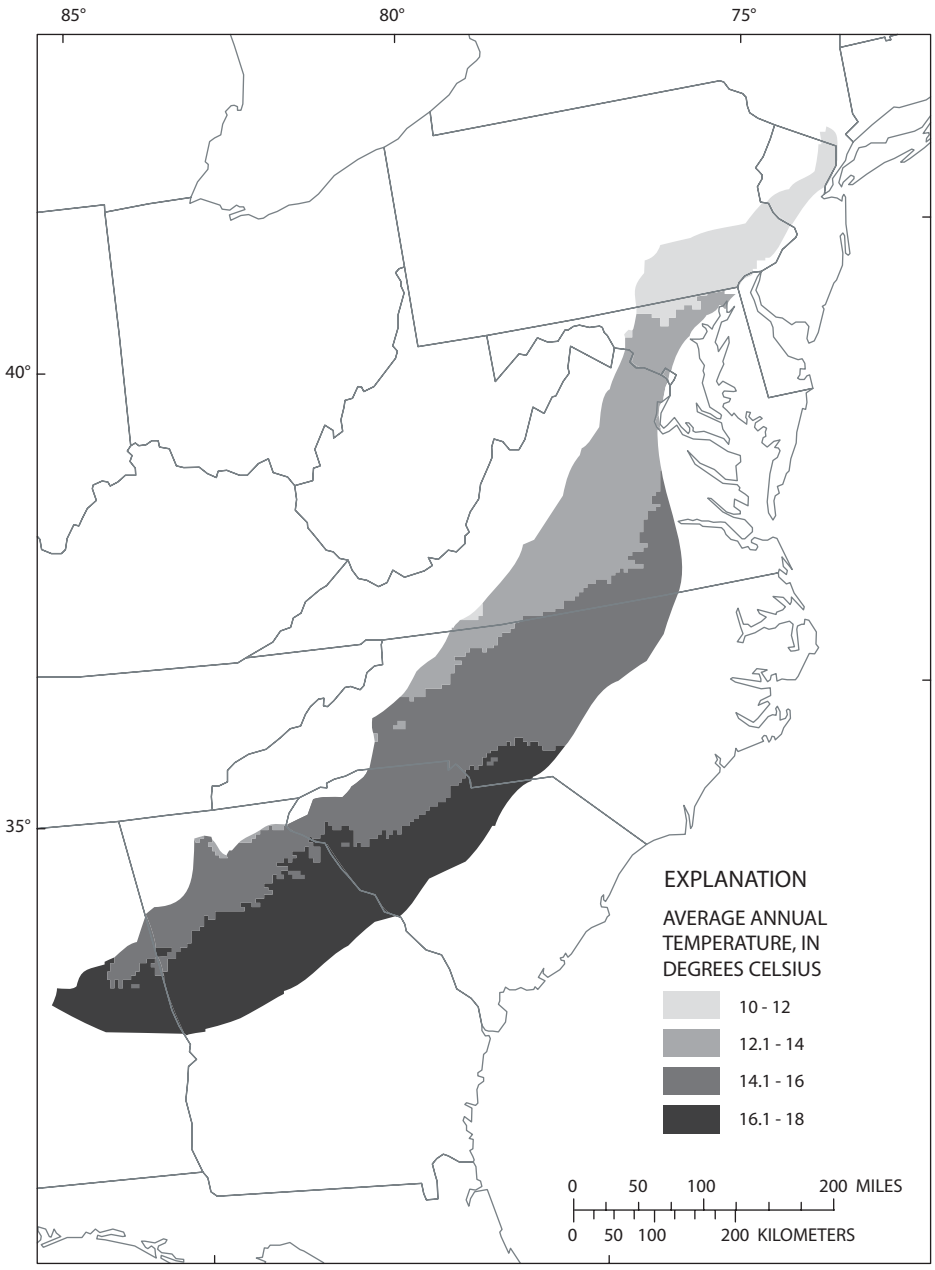

Figure 3. Average annual temperature in the Piedmont Aquifer System, eastern United States (from Falcone, 2004).

Precipitation

Precipitation ranges from less than 45 in/yr to more than 60 in/yr in the PAS (fig. 4) (Falcone, 2004). The higher rates of precipitation are related to topography, and the highest rates are in the mountainous regions of Georgia. Precipitation also increases somewhat from north to south; areas in the more humid south have higher rates of precipitation.

Recharge

Recharge is a function of precipitation, evapotranspiration, topography, and aquifer characteristics. The processes affecting recharge are complex and highly variable; however, a generalized summary of recharge in the PAS is illustrated in figure 5. Rutledge and Mesko (1996) reported a positive relation between precipitation and basin relief and recharge. In areas with similar evapotranspiration rates and aquifer characteristics, an area with greater relief and precipitation has higher recharge rates. The relation between precipitation and recharge can be seen by a comparison of precipitation (fig. 4) and recharge (fig. 5) in Georgia and South Carolina (Wolock, 2003). Highest recharge rates as a percentage of precipitation are in the carbonate-rock aquifer area of south-central Pennsylvania, and lowest recharge rates as a percentage of precipitation are in areas underlain by siliciclastic-rock aquifers (fig. 5).

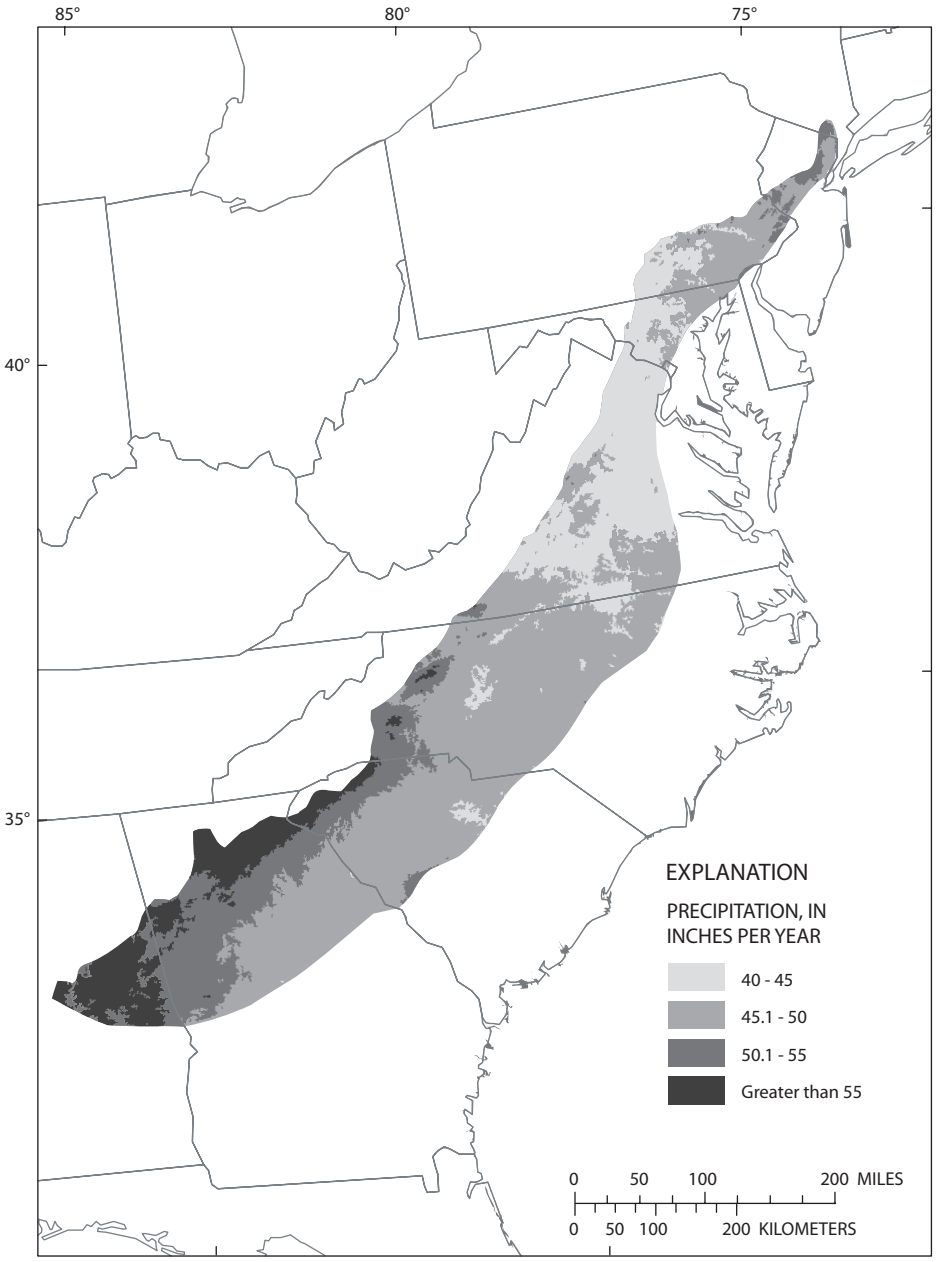

Figure 4. Average annual precipitation in the Piedmont Aquifer System, eastern United States (from Falcone, 2004).

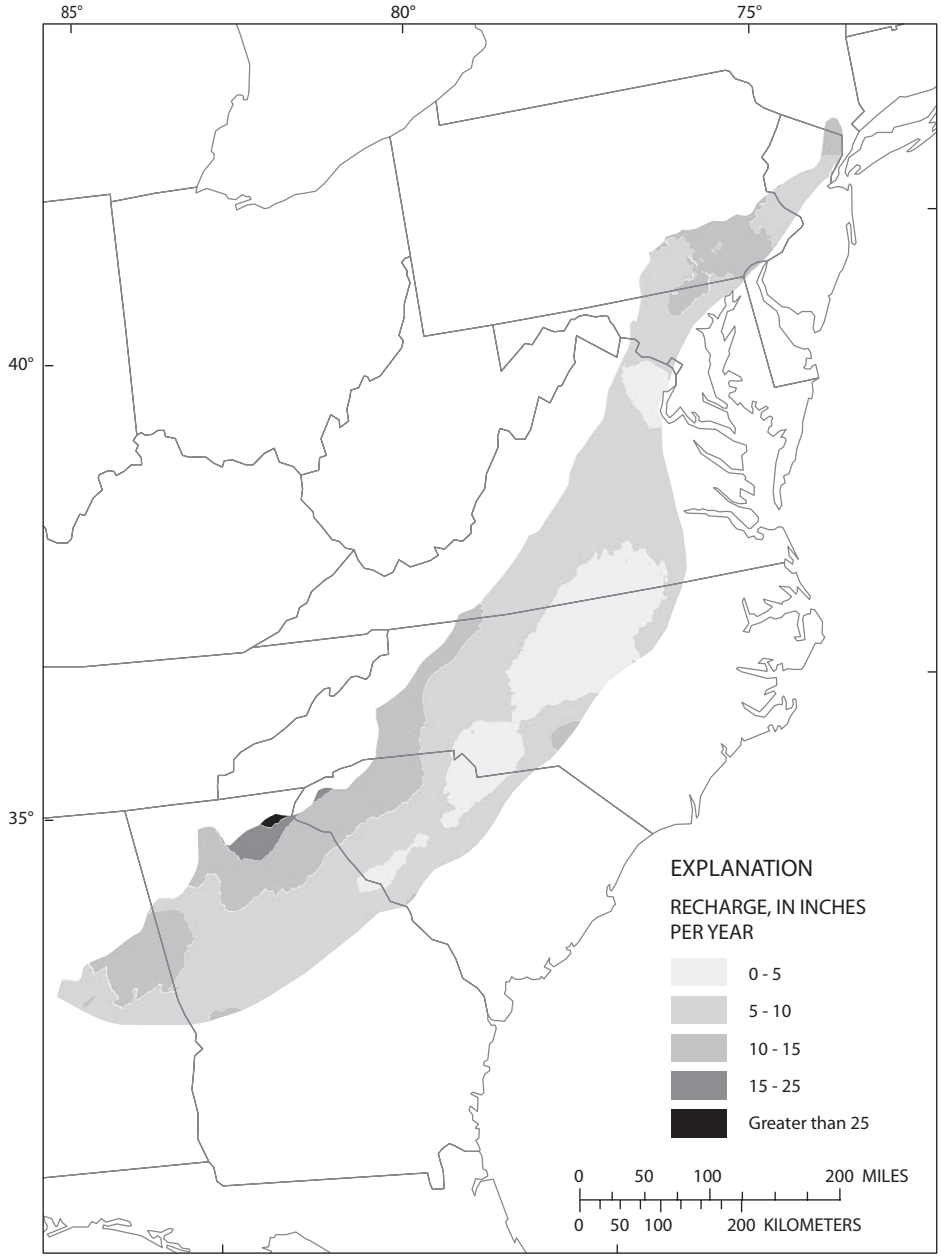

Figure 5. Average annual recharge in the Piedmont Aquifer System, eastern United States (from Wolock, 2003).

Description of Piedmont Aquifers and NAWQA Ground-Water Study Areas

The PAS is divided into the three basic aquifer types—crystalline, siliciclastic, and carbonate— for discussion of basic ground-water-flow systems. The characteristics of ground-water flow in the PAS are highly variable.

Crystalline-Rock Aquifers

The crystalline-rock aquifers underlie the largest part of the land area of the Piedmont Aquifer System (fig. 6). Crystalline bedrock includes a wide variety of igneous and metamorphic rocks that differ in origin, composition, and alteration. The lithologies include pelitic schist, coarse-grained felsic gneiss, mafic volcanic rocks, calcareous schist, granitoid plutonic rocks, greenstone, greenschist facies metabasalt, quartzite, mafic plutonic rocks (diorite, gabbro, mozodiorite, basalt), phyllite, and slate (Peper and others, 2001). The rocks are extensively folded, faulted, and fractured, commonly showing preferential joint orientation along fault zones and stress-relief fractures. Structure within the rocks, including bedding, foliation, and folding, also varies with rock origin and composition and is a factor in the susceptibility of rock weathering. The rocks are mantled by a cover of regolith, which is the unconsolidated material above competent bedrock and includes materials such as saprolite, colluvium, and alluvium. Generally, a zone of weathered rock, boulders, and saprolite are at the base of the regolith. This zone is referred to as the transition zone.

Hydrology

The hydrogeology of the Piedmont crystalline aquifer has been described by LeGrand (1967; 1992; 2004), Heath (1984, 1992), Swain and others (1991), and Daniel and Dahlen (2002). Small-scale studies of the crystalline-rock aquifers have been conducted by McFarland (1994) and Speiran (2003). The regolith and underlying fractured bedrock combine to make up a complex, multi-component ground-water-flow system. The components of the system are 1) the unsaturated zone in the regolith, 2) the saturated zone in the regolith, 3) the transition zone, and 4) the fractured-bedrock system (fig. 7). Recharge to the ground-water system is by infiltration of precipitation through the unsaturated zone. The regolith serves as a reservoir supplying water to interconnected fractures within the bedrock (Heath, 1980). The transition zone has high permeability relative to other zones, and it could create a high-flow zone within the ground-water-flow system (Harned and Daniel, 1992). The boundary of this transition zone with the fractured bedrock is irregular. The fractured-bedrock flow system has low storage capacity, yet where inter-connected fractures occur, water can move rapidly.

Ground-water recharge and discharge characteristics of the PAS were investigated by Rutledge and Mesko (1996) as part of the USGS Regional Aquifer System Analysis (RASA) study. The two components of streamflow—ground-water discharge and overland runoff—can be estimated for a given stream. If no long-term change in ground-water storage is assumed, ground-water discharge is equal to ground-water recharge. The ratio of base flow to total runoff is referred to by Rutledge and Mesko (1996) as the base-flow index. The median base-flow index for 10 streams in the southern Piedmont crystalline-rock aquifers is 44 percent of the total runoff (range = 65-32 percent; Harned and Daniel, 1987). Stream-discharge records were analyzed for streams in crystalline rocks in the Chesapeake Bay by Bachman and others (1998). They determined the average annual base-flow discharge for streams in this area was 8.5 in/yr. This translates to a median base-flow index of about 59 percent. The range, however, was from 25 to greater than 80 percent. Generally, ground water contributed over half of the total stream discharge.

In general, wells in the southern Piedmont crystalline-aquifer system are cased through the regolith and transition zone, with open hole through enough of the bedrock fractures to furnish acceptable yields. The bedrock fractures serve as pipelines between the well and the regolith reservoir (Heath, 1984).

Water Quality

Regional ground-water quality of the Piedmont was discussed by Harned (1989) and, as part of the RASA study, by Briel (1997) for major ions and nutrients. Water quality in the PAS also was described for smaller study areas by Clark and Stone (1992), Harned (1995), Daniel and others (1997), and Cunningham and Daniel (2001). The igneous and metamorphic rocks of the Piedmont crystalline-rock aquifers have few carbonate minerals; therefore, silicate weathering has a major effect on ground-water chemistry. This results in waters that have low concentrations of dissolved minerals and low pH. The mineral assemblages of the parent rock are reflected in the natural ionic composition of the ground water. Water from a granite aquifer generally will have a relatively high concentration of sodium bicarbonate, and ground water moving through mafic rock will have high magnesium and bicarbonate concentrations (Hem, 1985). Water from metavolcanic units may contain high iron concentrations. A study of ground water in the crystalline-rock aquifers in Pennsylvania indicated a median total hardness of 47 mg/L and a median pH of 6.0 (Taylor and Werkheiser, 1984). Statistics for 2,487 wells in North Carolina used in the USGS Appalachian Valleys-Piedmont RASA study (Briel, 1997; Harned, 1989) indicate a median of 6.6 for pH, 120 µS/cm for specific conductance, 40 mg/L for total hardness, 43 mg/L for total alkalinity, and 51 mg/L for bicarbonate. The median concentrations for iron and manganese were 0.10 mg/L and 50 µg/L, respectively.

Overlain on the natural water quality are surficial source and recharge influences of land use and land cover and anthropogenic sources of contamination. Harned (1989) found that the most predominant sources of contamination were landfills,

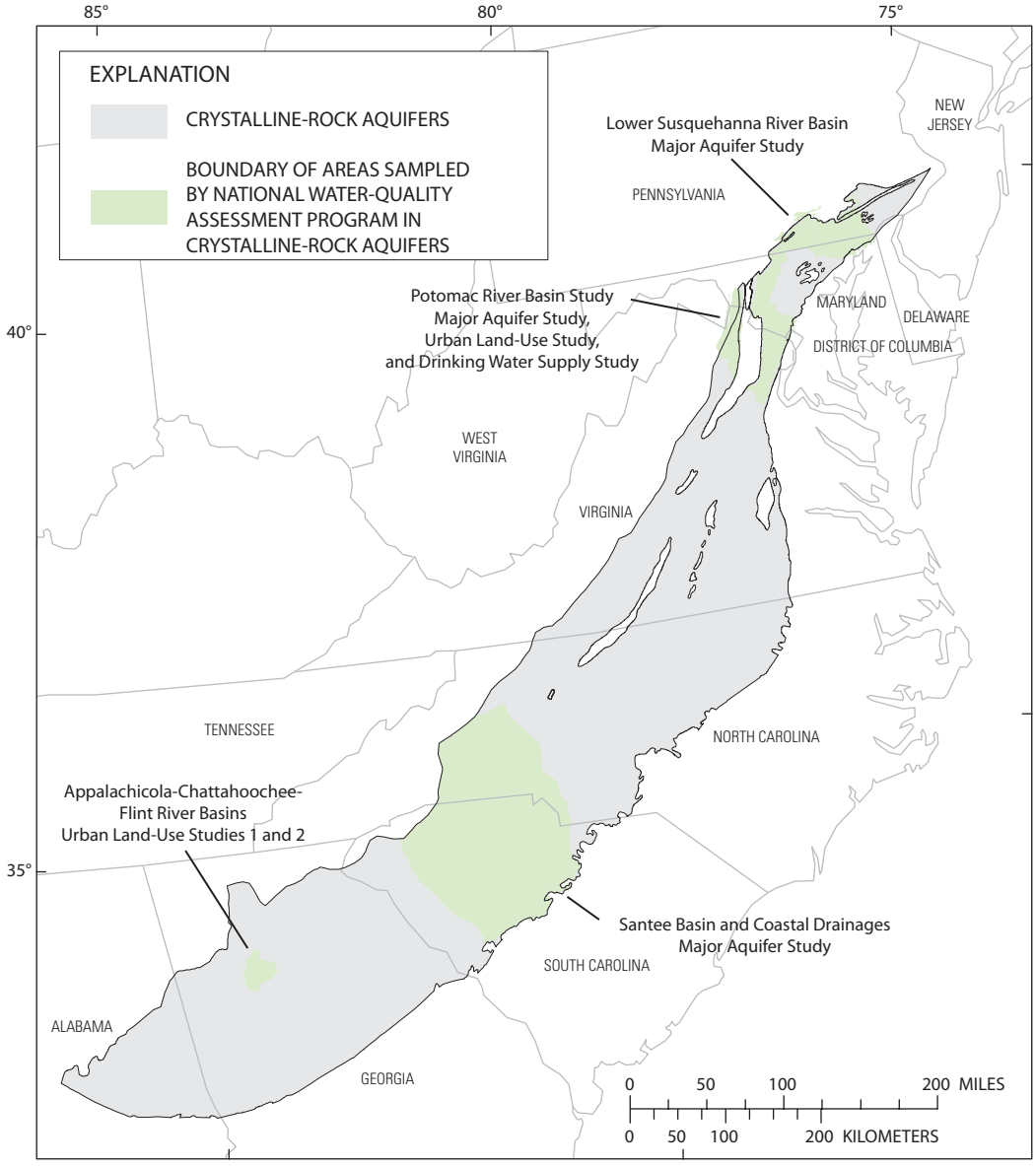

Figure 6. Location of areas sampled by the National Water-Quality Assessment Program in the crystalline-rock aquifers in the Piedmont Aquifer System, eastern United States.

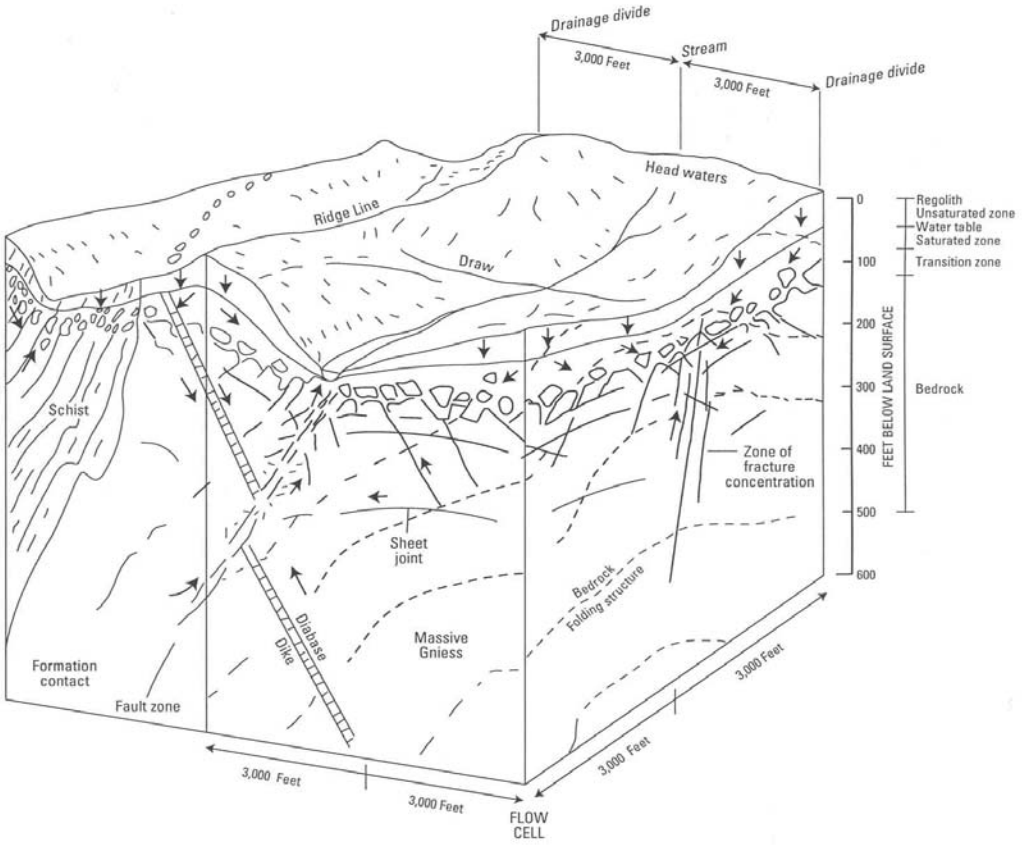

Figure 7. A conceptual representation of the Piedmont crystalline-rock aquifer flow system (modified from Harned and Daniel, 1992 and Daniel, 1990).

waste lagoons, fuel storage tanks, land application of wastewater, septic tanks, and spills. The median concentration for nitrite plus nitrate in crystalline-rock aquifers in North Carolina was 0.37 mg/L (Briel, 1997; Harned, 1989). Ground water associated with agricultural land uses had the highest median concentrations of nitrite plus nitrate (1.5 mg/L), followed by commercial (0.92 mg/L) and residential land uses (0.90 mg/L), all of which were considerably higher than ambient levels (0.16 mg/L) (Harned, 1989). A study of the Piedmont crystalline aquifer of the Lower Susquehanna River Basin by Hainly and Loper (1997) showed agricultural areas had a median nitrate concentration of 4.6 mg/L in ground water; the median nitrate concentration in forested areas was 1.6 mg/L.

NAWQA Studies in Crystalline-Rock Aquifers

The NAWQA Program conducted seven ground-water studies in the crystalline-rock aquifers of the PAS. The LSUS study unit conducted a major-aquifer study; the POTO study unit (later PODL study unit) conducted a major-aquifer study, an urban land-use study, and a drinking-water supply study in the crystalline-rock aquifers. The SANT study unit conducted a major-aquifer study, and the ACFB study unit conducted two urban land-use studies in the crystalline-rock aquifers, one of which sampled springs. In the 7 studies, 170 ground-water samples were collected. NAWQA studies cover about 14,500 mi^2 of the total area of about 86,500 mi^2 crystalline-rock aquifers or about 17 percent of the area.

Carbonate-Rock Aquifers

The carbonate-rock aquifers make up a small percentage of the land area of the PAS but are an important source of ground water in these areas. The carbonate-rock aquifers are found in northern New Jersey, southeastern Pennsylvania, and in central and eastern Maryland (fig. 8) (Trapp and Horn, 1997). The Piedmont carbonate-rock aquifers are predominantly Precambrian to lower Paleozoic age rocks. The geologic units in this area include limestone, dolomite, and marble. The carbonate rocks of the Piedmont have undergone several periods of deformation causing a complex structure of folds and faults. Although Trapp and Horn (1997) refer to these carbonate-rock aquifers as the Piedmont and Blue Ridge Carbonate Aquifer,

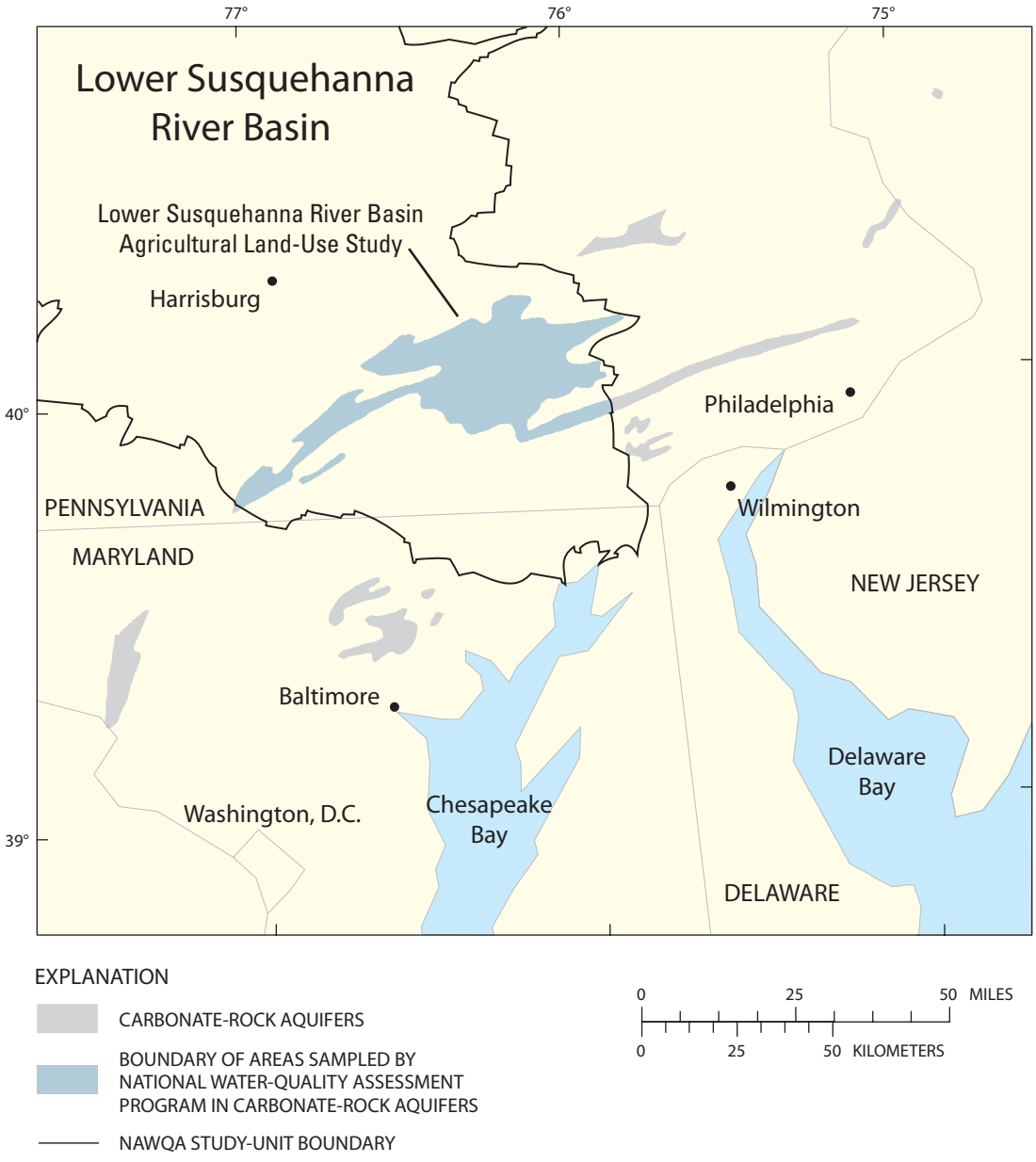

Figure 8. Location of areas studied by the National Water-Quality Assessment Program in the carbonate-rock aquifers in the Piedmont Aquifer System, eastern United States.

the Blue Ridge was not included in this study. Therefore, the area is referred to as the Piedmont carbonate-rock aquifers in this report.

Hydrology

Carbonate rocks are made up of highly soluble minerals, predominantly calcite (limestone rocks) and dolomite (dolomitic rocks). The dissolution of the carbonate bedrock typically occurs along structural planes such as bedding, cleavage, or other joints. Over time, these fractures are enlarged by the dissolution of the rock. These enlarged fractures range from horizontal to near-vertical depending on the orientation of the original fracture and the gradient of ground water toward the discharge point. Bedding planes typically have steep dip angles (fig. 9). The dissolution along fractures forms an inter-connected pattern of openings that greatly enhances permeability. In some cases, the openings are enlarged to the point at which turbulent flow occurs. Openings that are large enough to allow turbulent flow are called conduits, which have flow rates several orders of magnitude higher than flow rates in fractures. Because of the size of the solution channels in the weathered bedrock, ground water and contaminants can move rapidly through the ground-water system. The infiltration capacity of the soils is excellent (Susquehanna River Basin Study Coordinating Committee, 1970), which, combined with the flat terrain and conduits, makes internal drainage a common occurrence. The dissolution of carbonate rock also can cause formation of karst features such as sinkholes (fig. 9). Precipitation can flow into sinkholes or large fractures in the bedrock instead of running off into the streams, allowing contaminants to enter the aquifer with little or no filtration. The water then travels through large fractures, conduits, or caverns, discharging to the surface at springs and streams.

Well yields in the Piedmont carbonate-rock aquifers are highly variable. Yields in some of the geologic formations are poor; other formations have wells yielding over 1,800 gal/min (Low and others, 2002). Factors such as topography and lithology may affect well yield. Wells in valleys typically have higher yields, because these locations are likely to intersect major fracture sets and have a seasonal water table closer to the land surface. Wells in formations that include shaly units or more impure limestone may have lower well yields than those wells completed in more pure units.

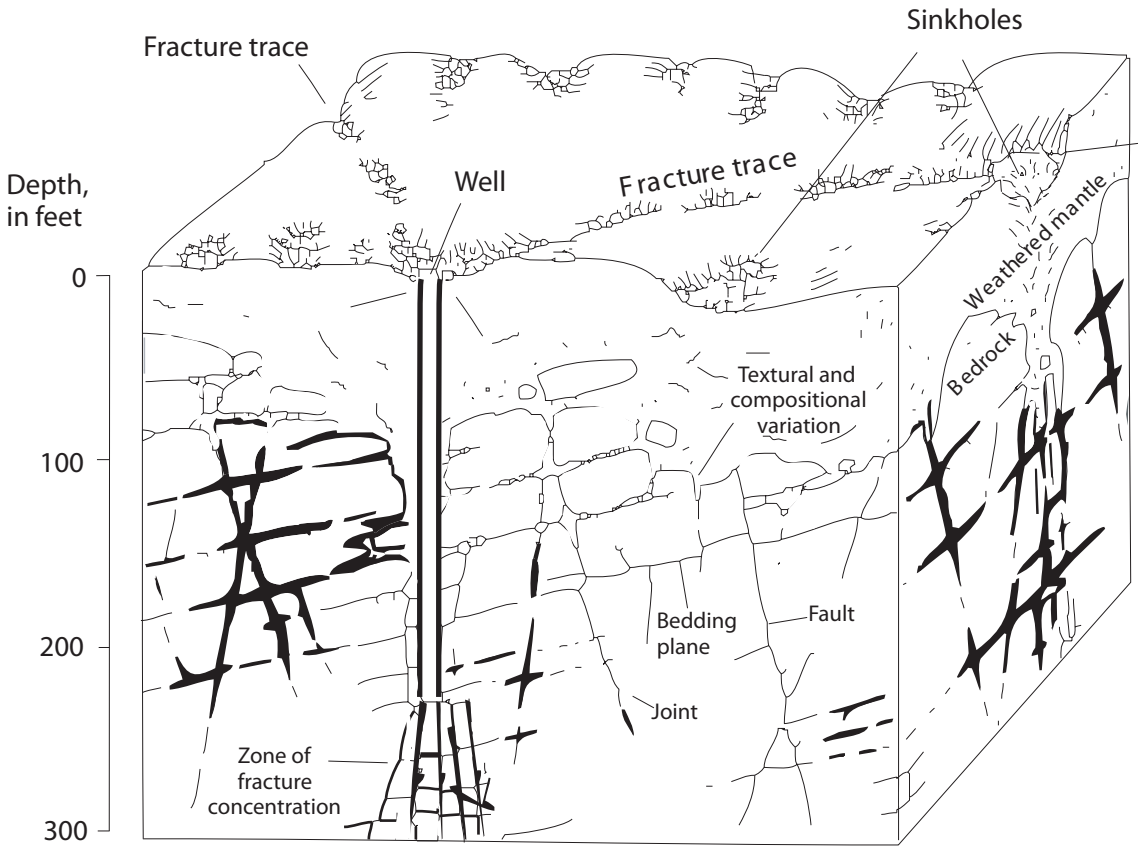

Figure 9. Hypothetical cross section of carbonate-rock aquifer in the Piedmont Aquifer System, eastern United States (modified from Lattman and Parizek, 1964).

In the area underlain by carbonate bedrock in the PAS, the base-flow index cannot be analyzed statistically because of the small number of streams. The only stream with long-term streamflow records that is predominantly in carbonate rock in the Piedmont is the Conestoga River at Conestoga (USGS station number 01576754), which had a median base flow of 11 in/yr and a base-flow index of 65 percent (Bachman and others, 1998). Bachman and others (1998) state that the base-flow index typically is higher in areas underlain by carbonate bedrock than in areas underlain by other bedrock types.

Water Quality

The weathering of the carbonate rocks results in water with high concentrations of dissolved solids. In an analysis of 361 wells in the Piedmont carbonate-rock aquifers (fig. 8), the median hardness was 264 mg/L and the median pH was 7.5 (Risser and Siwiec, 1996). The median hardness for this area is three times greater than the median hardness for the crystalline rocks in the same area. Hainly and Loper (1997) reported a median nitrate concentration of 9.2 mg/L in 173 wells in agricultural areas of the Piedmont carbonate aquifer and a median of 6.4 mg/L in 16 wells in urban areas of the Piedmont carbonate aquifer. Fishel and Lietman (1986) noted the occurrence of pesticides and the concentrations of nitrate were greater in water from wells in the carbonate aquifer of the PAS than in water from noncarbonate aquifers in the PAS.

NAWQA Studies in Carbonate-Rock Aquifers

The LSUS study unit conducted the only study of carbonate aquifers in the PAS (fig. 8). The study was an agricultural land-use study in which 30 domestic-supply wells were sampled. The area included in this land-use study covers about 450 mi^2 of the 900 mi^2 carbonate-rock aquifers in the PAS or about 50 percent of the land area.

Siliciclastic-Rock Aquifers

Siliciclastic aquifers of Early Mesozoic Age are found in a discontinuous belt from Massachusetts to South Carolina; these aquifers are interspersed with intrusions of crystalline rocks such as diabase. The siliciclastic-rock aquifers within the PAS are illustrated on figure 10. Horton and Zullo (1991) described some geologic basins as having three sequences: a lower sequence of reddish-brown, coarse-grained arkose and conglomerate; a middle sequence of gray to black fossiliferous siltstone, carbonaceous shale, and thin coal beds; and an upper sequence of reddish-brown siltstone, arkose, pebbly sandstone, minor red and gray mudstone, and conglomerate. Facies within the geologic basins change rapidly, both vertically and laterally (Bain and Brown, 1981). Most strata within the geologic basins dips between 5 and 40 degrees toward the main border fault (Horton and Zullo, 1991; Swain and others, 1991). Diabase dikes and sills are common in the basins. The dikes in North Carolina range from a few feet to several hundred feet in width and have nearly vertical dips (Mundorff, 1948; Horton and Zullo, 1991). As previously stated, the diabase parts of the PAS were not sampled; therefore, this area is referred to as the Piedmont siliciclastic-rock aquifers in this report.

Hydrology

In the Piedmont siliciclastic-rock aquifers, ground-water flow is primarily through a network of fractures, joints, bedding planes, and faults (fig. 11). To a lesser extent, flow is through interstitial pore space and solution channels (Daniel and Dahlen, 2002). The formations have little primary porosity, less than 5 percent in most cases, because of poor sorting of the sediment and secondary compaction and cementation (Nutter, 1975). The capacity of the siliciclastic-rock aquifers to store and transmit water tends to decrease with depth because the weight of the overlying strata closes fractures (Herpers and Barksdale, 1951). Depth of the overburden appears to have little relation to well yield in the siliciclastic-rock aquifers (Bain and Thomas, 1966). Ground-water flow is anisotropic in some basins, favoring the strike direction of the bedding or major joint set (Herpers and Barksdale, 1951; Nutter, 1975; Swain and others, 1991).

Well yields in the siliciclastic-rock aquifers decrease from north to south; well yields in the Durham, Sanford, and Wadesboro subbasins in North Carolina are among the lowest of all aquifers in the PAS (Swain and others, 1991). Studies indicated well yields of up to 500 gal/min in the Newark, N.J., area (Herpers and Barksdale, 1951) and up to 1,500 gal/min in the fractured shale and sandstone aquifer of northern Virginia, Pennsylvania, and New Jersey (Daniel and Dahlen, 2002). Most other studies indicated well yields ranging from 5 to 25 gal/min (Nutter, 1975; Mundorff, 1948; Schipf, 1961; Bain and Thomas, 1966); the higher yields were in coarse-grained rocks such as the limestone-pebble conglomerate of the siliciclastic-rock aquifers in Maryland, and lower yields were in fine-grained rocks of the Deep River Basin, N.C. Higher yields also have been reported for wells in valleys and wells near faults. Areas around faults can be severely sheared and fractured (Nutter, 1975). The base-flow index in areas underlain by siliciclastic bedrock was 5.9 in/yr, which was a statistically significant lower median value than in areas underlain by other bedrock types in the Chesapeake Bay (Bachman and others, 1998).

Water Quality

In the siliciclastic-rock aquifers of the PAS, regional differences in water chemistry reflect regional differences in rock mineralogy and texture and ground-water residence times (Daniel and Dahlen, 2002). Swain and others (1991) reported that ground water generally is hard (greater than 120 mg/L calcium carbonate ($CaCO_3$)) to very hard (greater than 180 mg/L $CaCO_3$) in the Piedmont siliciclastic aquifer. This is several times greater than the hardness in the crystalline-rock aquifer,

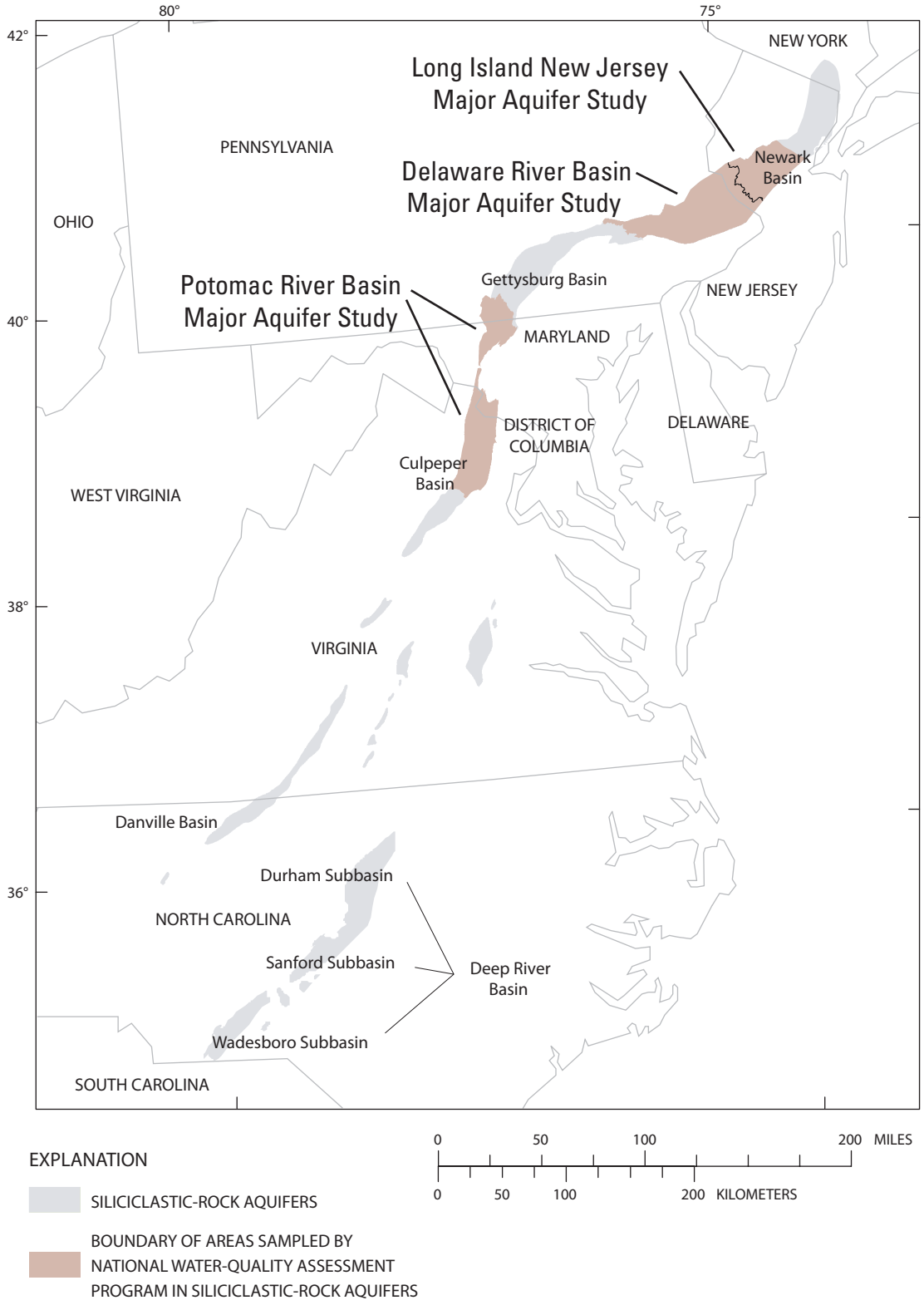

Figure 10. Location of areas studied by the National Water-Quality Assessment Program in the siliciclastic-rock aquifers in the Piedmont Aquifer System, eastern United States.

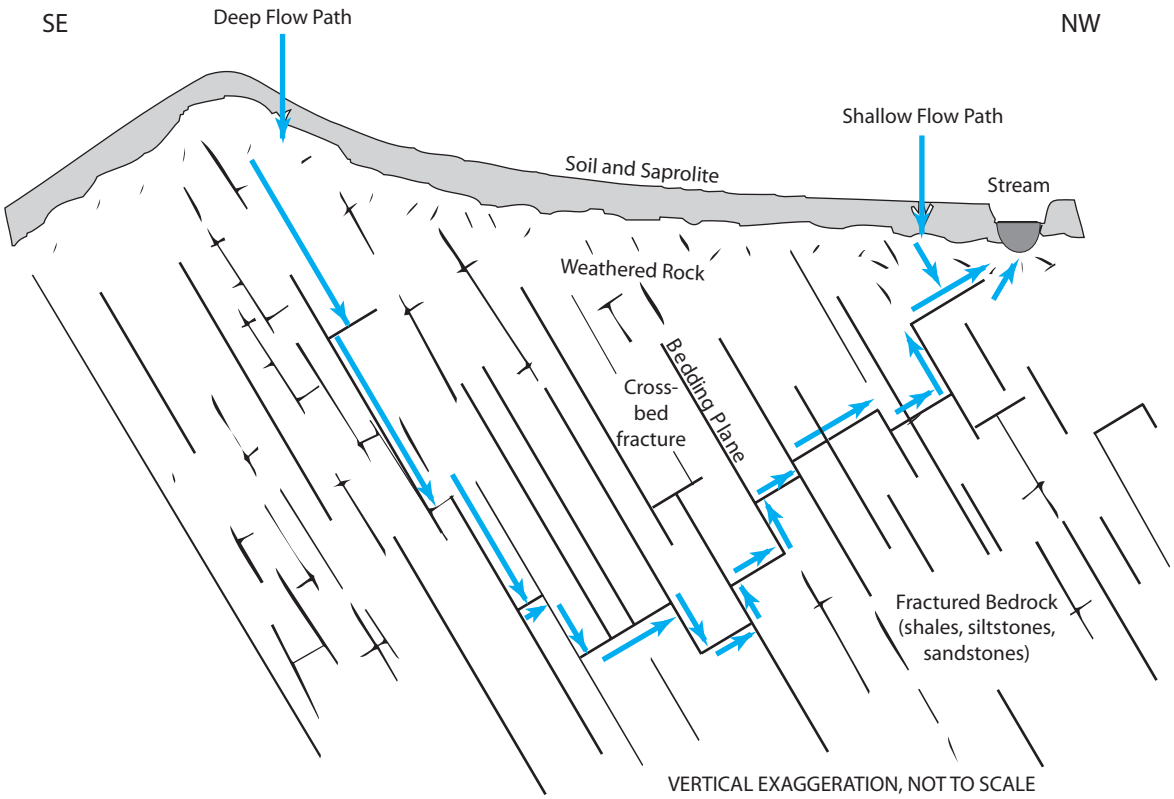

Figure 11. Hypothetical cross section of siliciclastic aquifer in the Piedmont Aquifer System, eastern United States (modified from Goode and Senior, 2000).

and in the same range of hardness in the carbonate-rock aquifer. Concentrations of iron and manganese may be locally elevated in the ground water. In Maryland, 18 percent of well samples had concentrations of iron greater than 0.30 mg/L, and concentrations of manganese exceeded 50 µg/L in 13 percent of the well samples (Nutter, 1975). In the Durham Basin in North Carolina, dissolved solids in ground water generally were less than 250 mg/L (Brown, 1988). Water samples from wells completed in siliciclastic bedrock had median concentrations of 0.15 mg/L for iron, 158 mg/L for hardness, and 75 mg/L for chloride.

NAWQA Studies in Siliciclastic-Rock Aquifers

Three NAWQA Program study units conducted sampling in the siliciclastic-rock aquifers of the PAS: the LINJ, the DELR, and the POTO study units (fig. 10). All three of these studies were major-aquifer studies; therefore, no particular land-use type was targeted. Wells sampled were primarily domestic-supply wells. In the 3 studies, 74 wells were sampled. The area covered by these three studies is about 3,100 mi^2, which is about half the area of the entire siliciclastic-rock aquifers (6,000 mi^2).

Description of NAWQA Well Networks

The NAWQA Program conducts assessments of both ground-water and surface-water quality in more than 50 study units throughout the nation. Nine NAWQA study units include parts of the PAS. Each study unit selects areas within their respective study unit for focused ground-water studies. Six of the nine study units conducted ground-water studies in the PAS. Because some study units conducted more than one study within the PAS, a total of 11 studies were conducted in those 6 study units. These ground-water studies fall into three major categories. These categories are major-aquifer studies, land-use studies, and drinking-water studies. A major-aquifer study (MAS) is intended to characterize the water quality in a major aquifer within a study unit, without regard to land use. Typically, the well network for a MAS includes mostly domestic-supply wells. Early NAWQA studies referred to these studies as a subunit survey (SUS). Another study type is called a land-use study (LUS). This is similar to a MAS in that it is focused on aquifers representing a specific rock type within a study unit; however, sample locations are selected to represent the shallow water-bearing zones of aquifers underlying a specific land-use type. In the well network for a LUS, the wells may be domestic-supply wells, if the domestic wells are considered to be representative of the shallow ground-water system. If domestic wells are too deep or not available, other well types are sampled for the LUS. These wells can be existing monitor wells, monitor wells drilled specifically for the project, or unused wells. The two types of land-use studies were agricultural and urban. An agricultural land-use study is designed to determine quality of shallow ground water in areas where land use is predominantly agricultural, such as row crops and pasture. The urban land-use studies are designed to determine ground-water quality near industrial, commercial, or residential land uses. The third type of study is a drinking-water-supply study (DWS), in which public water supplies are sampled within a given aquifer. The well network for a DWS typically includes wells that are deeper than in the other networks. A description of the locations, numbers of wells sampled, and types of studies for each of the well networks is shown in table 2. The locations of the 11 ground-water study areas and the locations of the wells sampled are shown in figures 12 and 13. In the POTO study unit, a MAS, a DWS, and an urban LUS overlap. Abbreviations for the 11 ground-water study areas used in this report include the NAWQA study unit; type of study; in some cases, land use; and a numeric designation (table 2). For example, *acfblusur1* is the Appalachicola-Chattahooche/Flint River Basin NAWQA study unit (acfb), land-use study (lus) of urban areas (ur), and it is the first study (1) of this area. The number of samples collected for a given constituent varied slightly among study units because of design issues, budgets, and occasional missing samples. A summary of the constituents sampled within each network is given in table 3.

Table 2. Descriptions of ground-water study areas sampled in the Piedmont Aquifer System.

[LUS, land-use study; MAS, major-aquifer study; DWS, drinking-water-supply study]

Ground-water study-area code	Study unit and abbreviation	Type of study	Aquifer type	Aquifer lithology	Type of aquifer media	Map of well locations
acfblusur1	Appalachicola-Chattahooche Flint River Basin (ACFB)	Urban LUS	Crystalline	Saprolite/Igneous and metamorphic rocks	Unconsolidated porous medium	Fig. 13
[1]acfblusur2	Appalachicola-Chattahooche Flint River Basin (ACFB)	Urban LUS	Crystalline	Saprolite/Igneous and metamorphic rocks	Unconsolidated porous medium	Fig. 13
delrsus1	Delaware River Basin (DELR)	MAS	Siliciclastic	Sandstone and shale	Fractured bedrock	Fig. 12
linjsus3	Long Island/New Jersey (LINJ)	MAS	Siliciclastic	Sandstone and shale	Fractured bedrock	Fig. 12
lsuslusag1	Lower Susquehanna River Basin (LSUS)	Agricultural LUS	Carbonate	Limestone and dolomite	Fracture and conduit flow	Fig. 12
lsussus2	Lower Susquehanna River Basin (LSUS)	MAS	Crystalline	Igneous and metamorphic rocks	Fractured bedrock	Fig. 12
podllusrc1	Potomac/Delmarva (PODL)	LUS	Crystalline	Igneous and metamorphic rocks	Fractured bedrock	Fig. 12
podldwgs1	Potomac/Delmarva (PODL)	DWS	Crystalline	Igneous and metamorphic rocks	Fractured bedrock	Fig. 12
potosus1	Potomac/Delmarva (PODL)—formerly Potomac River Basin	MAS	Crystalline	Igneous and metamorphic rocks	Fractured bedrock	Fig. 12
potosus2	Potomac/Delmarva (PODL)	MAS	Siliciclastic	Sandstone and shale	Fractured bedrock	Fig. 12
santsus3	Santee River Basin (SANT)	MAS	Crystalline	Igneous and metamorphic rocks	Fractured bedrock	Fig. 13

[1]Springs were sampled for acfblusur2

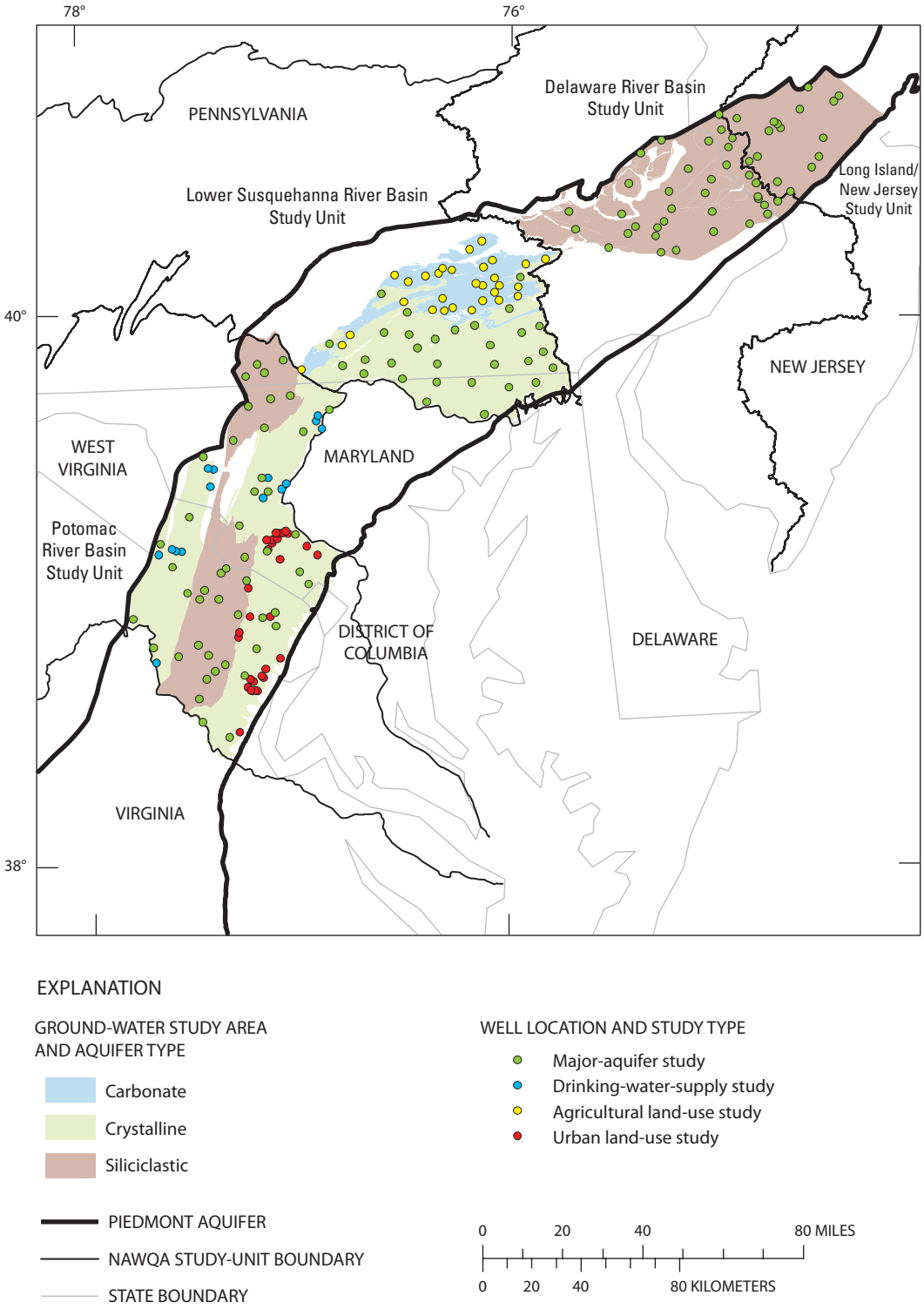

Figure 12. Locations of ground-water study areas and wells sampled in the northern area of the Piedmont Aquifer System, eastern United States.

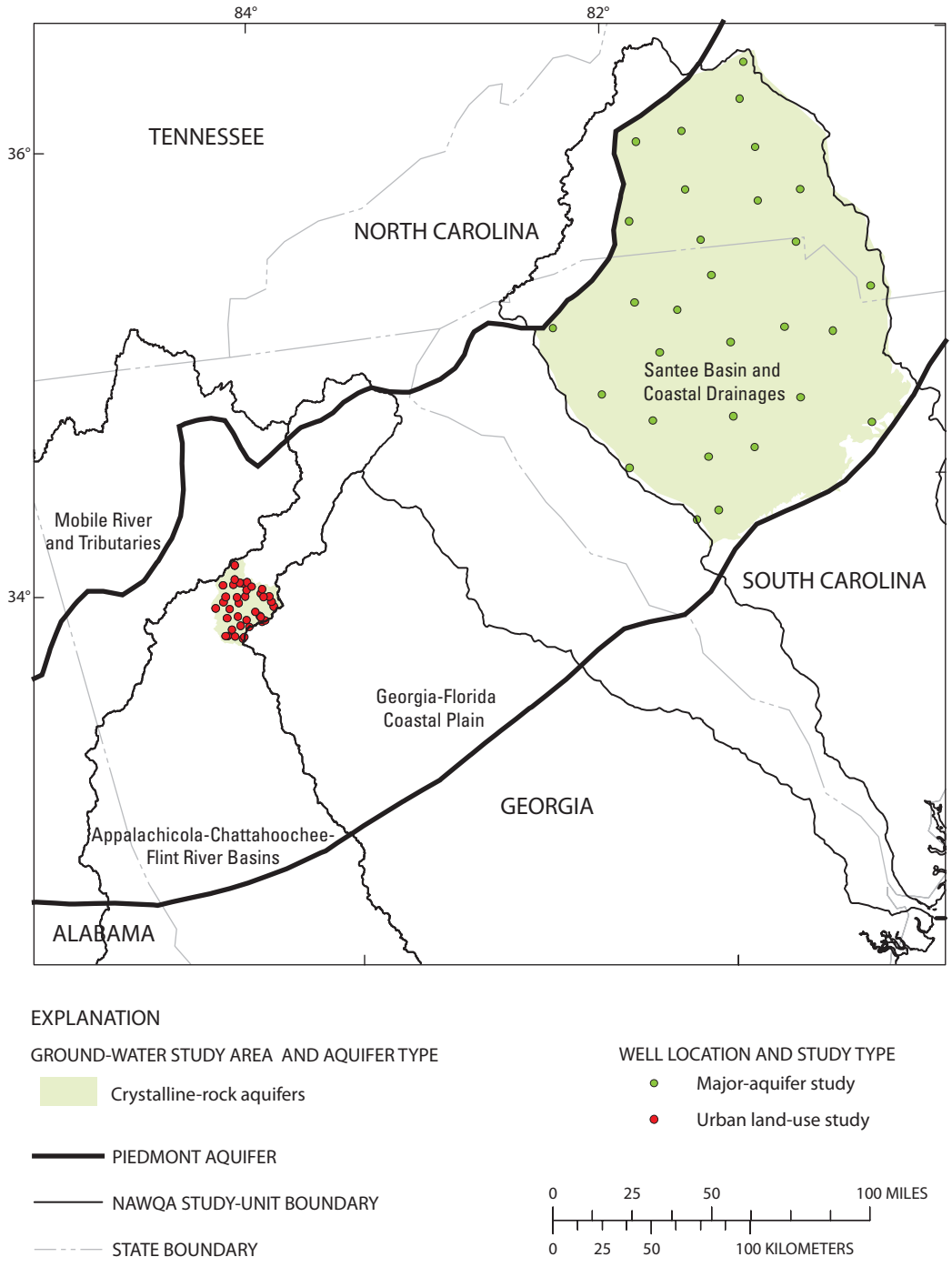

Figure 13. Locations of ground-water study areas and wells sampled in the southern area of the Piedmont Aquifer System, eastern United States.

Table 3. Summary of major constituents sampled in ground-water study areas in the Piedmont Aquifer System.

Ground-water study-area code	Constituent group and number of samples					
	Number of wells	Nutrients	Pesticides	Volatile organic compounds	Radon	Trace elements
[1]acfblusur1	21	21	20	21	21	21
acfblusur2	[2]19	19	17	19	18	19
delrsus1	30	30	30	30	30	30
linjsus3	21	21	20	21	0	21
lsuslusag1	30	30	30	30	29	0
lsussus2	30	30	30	10	29	0
podllusrc1	30	30	30	30	0	30
podldwgs1	15	0	15	15	0	0
potosus1	25	25	25	0	25	0
potosus2	23	23	23	0	23	0
santsus3	30	30	30	30	30	30
Total samples	274	259	270	206	205	151

[1]Ground-water study-area codes are defined on table 2.

[2]Springs were sampled for this study.

Physical Characteristics of Wells and Surrounding Areas

The results of water-quality sampling can be affected by many factors related to the physical characteristics at or near a well. These factors include the aquifer in which the well is completed, the land use surrounding the well, soils, climate, and characteristics of the construction of the well.

The factors that affect ground-water quality include availability of contaminant sources and aquifer susceptibility. The aquifer lithology affects the ease with which contaminants can enter an aquifer. In these studies, wells were selected on the basis of the bedrock type in which they are completed, and therefore, one bedrock type is associated with a given well or study area (table 2). The type of media, however, is not necessarily the same for all bedrock types. For example, some wells in the crystalline-rock aquifer are completed in fractured bedrock and others are completed in saprolite. Therefore, both the aquifer lithology and type of media are considered to be factors potentially affecting water quality. In the case of some contaminants, such as radon, the minerals in the aquifer are also the source of the contaminant.

The physical characteristics of individual wells are related to the aquifer characteristics and the purpose of the wells. A summary of well depth, casing length, and water level is shown in figure 14. The two urban land-use studies (acfblusur1 and podlusrc1) that used monitor wells had the shallowest depths, casing lengths, and water levels. These wells typically were completed in the shallowest water-bearing zones. The drinking-water-supply study (podldwgs1) had the deepest well depths and casing lengths. Public-supply wells typically are drilled deeper than monitor wells or domestic-supply wells, and shallow water-bearing zones commonly are cased off to reduce susceptibility to surface contamination. The remaining wells are all domestic-supply wells and had a similar range of characteristics of construction. The wells in the santsus3 study had the longest casing lengths and deepest wells of all the domestic-supply well studies.

Other data also are available to describe the physical setting in which each well is located. The USGS NAWQA Program summarized ancillary data for a 1,640-ft (500-m) radius around each well for national synthesis projects, and therefore, selected ancillary data had already been compiled for all NAWQA wells for that radius. Soils data from State Soil Geographic Data (STATSGO, U.S. Department of Agriculture, 2003) was analyzed for the 1,640-ft radius. This arbitrary radius was assumed to be related to, but not necessarily the same as, the recharge area of the well. This data set includes characteristics such as permeability, soil thickness, organic-matter content, particle size, and hydrologic groupings (table 4) and will be used to explain water-quality results. Hydrologic groups are ordered from A to D with the A having the lowest runoff potential and D having the highest runoff potential (U.S. Department of Agriculture, 1986).

Land use differs within each ground-water study area and among individual wells. Land uses around a well affect potential sources of contaminants that could be present, and these data have been compiled for each ground-water study area and for a 1,640-ft radius around each well (table 5) (Vogelmann and

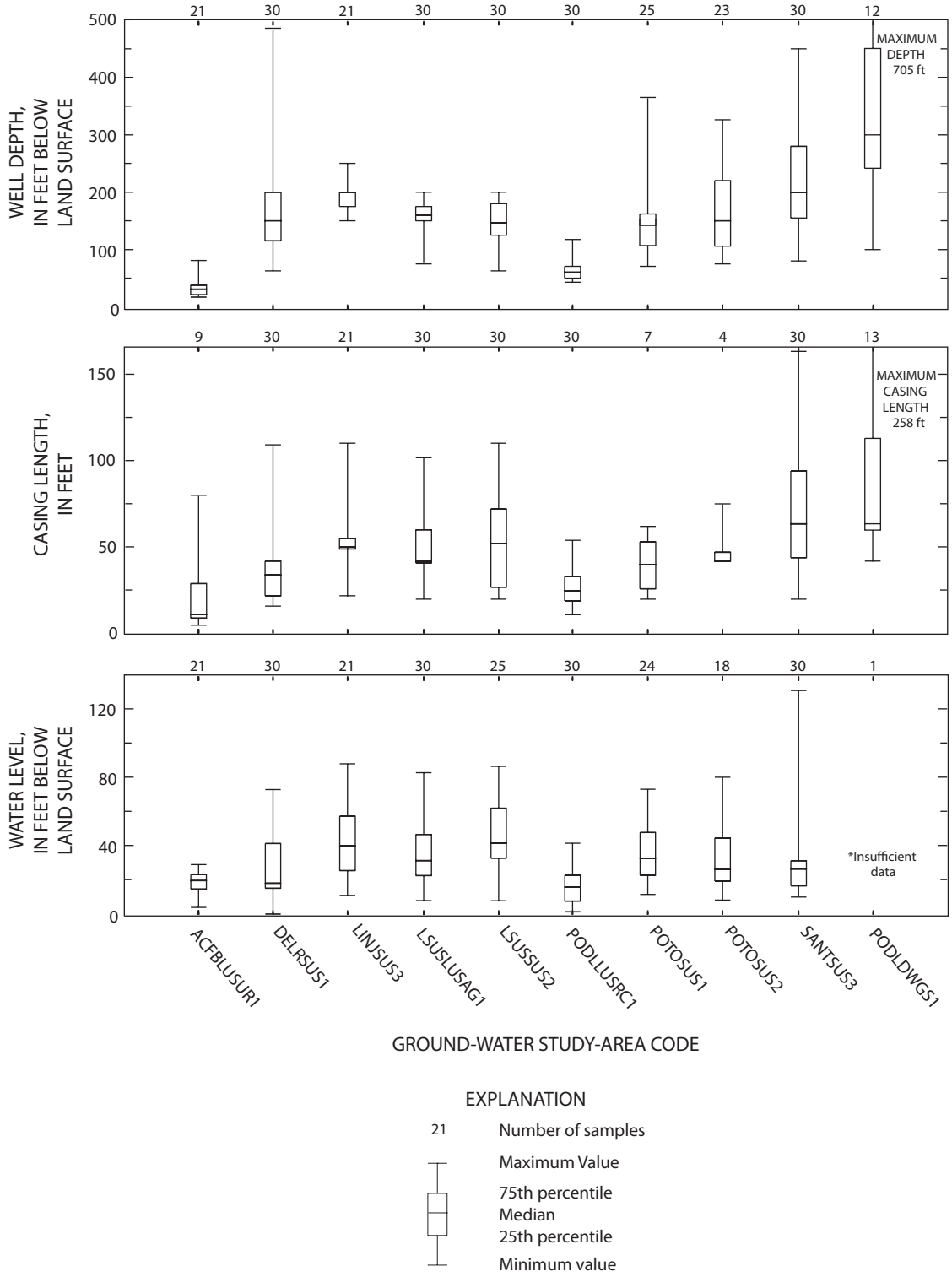

Figure 14. Well depths, casing lengths, and water levels for well networks in the Piedmont Aquifer System. (Ground-water study-area codes are defined on table 2. ACFBLUSUR2 not shown because network was springs.)

Table 4. Summary of soil characteristics within a 1,640-ft radius of wells and springs in ground-water study areas in the Piedmont Aquifer System.

Ground-water study-area code	STATSGO Soil characteristics[1]									
	Median percentage of area in hydrologic group				Median value for		Median percentage soil content of			
	A	B	C	D	Soil thickness (inches)	Permeability (inches per hour)	Organic matter	Clay	Silt	Sand
[2]acfblusur1	0	100	0	0	33.7	106	0.3	35.8	29.9	34.3
acfblusur2	0	100	0	0	33.7	1.6	.3	35.8	29.9	34.3
delrsus1	0	36	49	5	48.6	2.0	.6	20.1	50.9	29.0
linjsus3	0	32	65	3	45.6	2.4	.8	21.3	54.1	24.3
lsuslusag1	0	84	14	0	64.4	1.4	.6	36.1	54.4	9.5
lsussus2	6	77	9	7	55.7	1.6	.5	19.8	53.2	27.1
podllusrc1	0	78	13	3	51.1	2.0	.5	25.5	48.9	30.2
podldwgs1	0	76	8	2	51.1	2.4	.5	21.6	40.7	36.1
potosus1	4	78	8	3	51.1	2.3	.5	21.6	42.0	36.1
potosus2	0	9	49	10	46.1	2.3	.7	22.8	50.0	24.9
santsus3	0	87	12	0	54.5	1.5	.4	35.1	31.1	32.8

[1]U.S. Department of Agriculture (2003).

[2]Ground-water study-area codes are defined on table 2.

Table 5. Summary of land use in ground-water study areas sampled by NAWQA study units in the Piedmont Aquifer System.

[NA, not applicable]

Ground-water study-area code	Type of land-use study	Land use within ground-water study area (percent)[1]			Land use within 1,640-ft radius of wells and springs (percent, mean for all wells)		
		Urban	Forested	Agricultural	Urban	Forested	Agricultural
[2]acfblusur1	Urban	87	12	0	57	17	0
[3]acfblusur2	Urban	87	12	0	58	33	0
delrsus1	NA	18	40	38	36	25	39
linjsus3	NA	29	38	31	1	26	34
lsuslusag1	Agricultural	3	6	89	0	2	97
lsussus2	NA	3	34	59	0	19	77
podllusrc1	NA	20	36	41	5	11	53
podldwgs1	Urban	26	48	17	19	37	10
potosus1	NA	20	36	41	5	22	46
potosus2	NA	12	33	51	0	19	65
santsus3	NA	10	65	19	0	80	17

[1]Vogelmann and others (1998a, 1998b).

[2]Ground-water study-area codes are defined on table 2.

[3]Springs were sampled for this study.

others, 1998a, 1998b). Land-use practices related to the application of nitrogen are considered to potentially affect nitrate concentration. These land uses would include row crop/pasture and hay (fertilizer and manure) and commercial/residential (home fertilizer use, leading sewage lines, and private septic systems). Similarly, agricultural application of herbicides would be expected to affect herbicide concentrations, and urban application of certain insecticides would be expected to affect insecticide concentrations. Urban uses and releases of VOCs can potentially affect VOC concentrations. The summary of land-use types in table combines row crop and pasture and hay into a category called agricultural. The categories of high-density residential, low-density residential, and commercial/industrial are combined into a category called urban. Deciduous, coniferous, and mixed forests are combined into a category called forested. A summary of the predominant land uses in the ground-water study area and the typical land use around individual wells is given in table 5. In most cases, the distribution of land use around the wells in the network is representative of the land use in the ground-water study area it is in.

Although ancillary data are available to assess the factors affecting ground-water quality, it is important to note that these studies were developed independently for priorities of each individual study unit and not to conduct an overall assessment of the PAS. In some cases the full spectrum of potential water-quality issues has not been fully explored (table 6). It is because of the gaps in this matrix that the analysis of these data are deemed to be for the study areas only and not necessarily representative of all the PAS.

Chemical Characteristics of Natural Ground Water

The natural chemistry of water can be important in understanding the presence or concentrations of contaminants in an aquifer. The mobility and degradation of contaminants can be affected by characteristics such as pH and dissolved oxygen concentrations. Natural chemistry and water characteristics (figs. 15 and 16) collected from each of the well networks is presented in order to establish basic aquifer characteristics for each network and illustrate similarities and differences among aquifers.

The field characteristics (fig. 15) illustrate water from the wells in the carbonate-rock aquifers tended to have a median pH near 7.0 and a very narrow range of pH values. Wells in the siliciclastic-rock aquifers had a median pH near 7.0 but a greater range of pH values. Wells in the crystalline-rock aquifers had water with a median pH closer to 6.0 and the largest range of pH values. This pattern is consistent with what would be expected; water from the well network in the carbonate-rock aquifers is well buffered as a result of the dissolution of calcite, and the water from well networks in the crystalline-rock aquifers is acidic and poorly buffered as a result of silicate weathering. The water from wells in the siliciclastic-rock aquifer have a broad range of values of pH and alkalinity, which is based on the presence or absence of carbonate cement in the siliciclastic rocks. Specific conductance follows a similar pattern; water from the carbonate aquifer had the highest median specific conductance, water from the networks in the crystalline aquifers had the lowest median values of specific conductance, and water from the siliciclastic aquifer had median values in the middle of that range.

Table 6. Summary of wells sampled within the Piedmont Aquifer System by combination of well type and land use.

Well type and land use	Number of samples in aquifer type		
	Carbonate	Crystalline	Siliciclastic
Shallow agricultural land use	0		
Domestic agricultural land use	30	None	None
Water-supply agricultural land use	0		
Shallow urban land use		70	
Domestic urban land use[1]	None	0	None
Water-supply urban land use		0	
Shallow forested land use			
Domestic forested land use	None[2]	None	None
Water-supply forested land use			
Shallow mixed land use		0	0
Domestic mixed land use	None	85	74
Water-supply mixed land use		15	0

[1]Establishing a domestic well network in an urban area is improbably because of lack of existing wells in areas already on public water supply.

[2]Forest land makes up less than 2 percent of the carbonate-rock aquifer in the Piedmont Aquifer System.

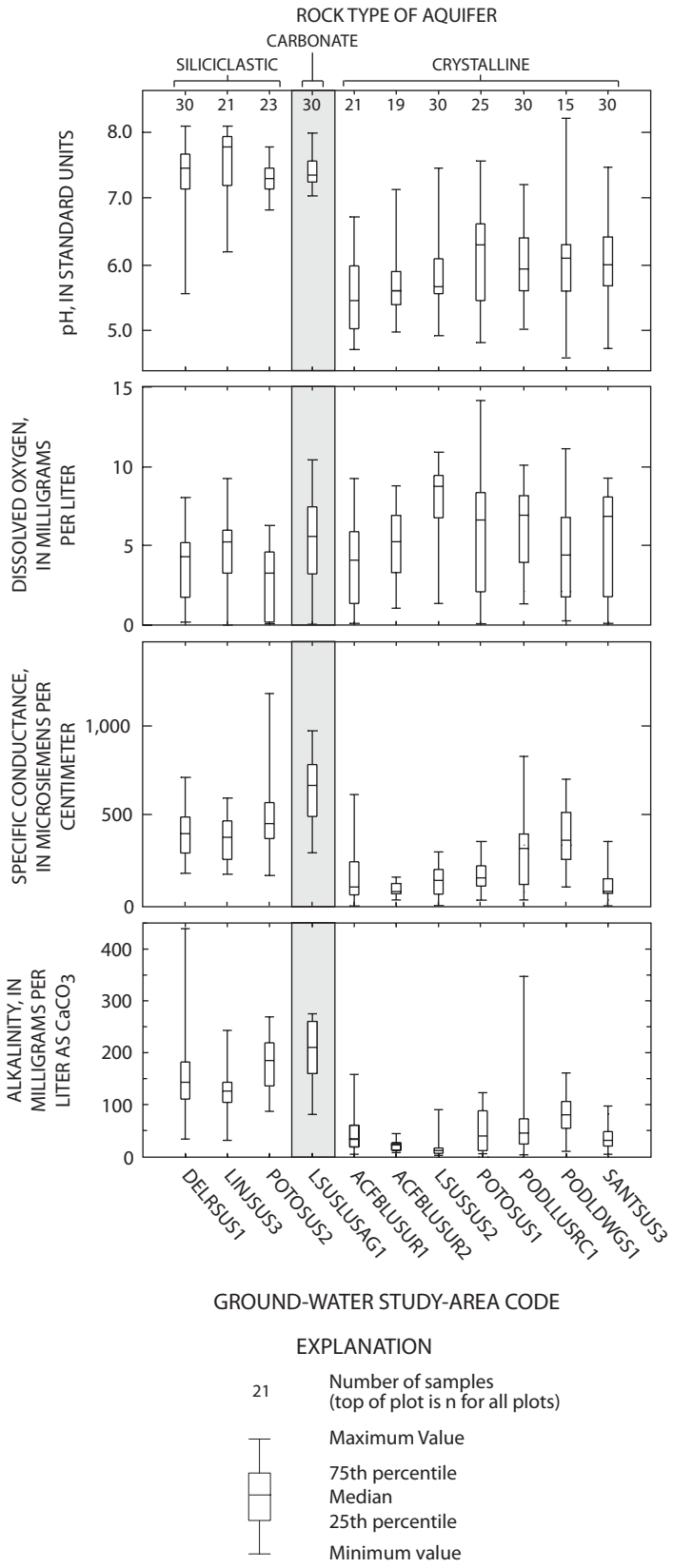

Figure 15. Summary of pH, dissolved oxygen, specific conductance, and alkalinity measurements for ground-water samples collected by the USGS NAWQA Program from ground-water study areas in the Piedmont Aquifer System, eastern United States. (Ground-water study-area codes are defined in table 2.)

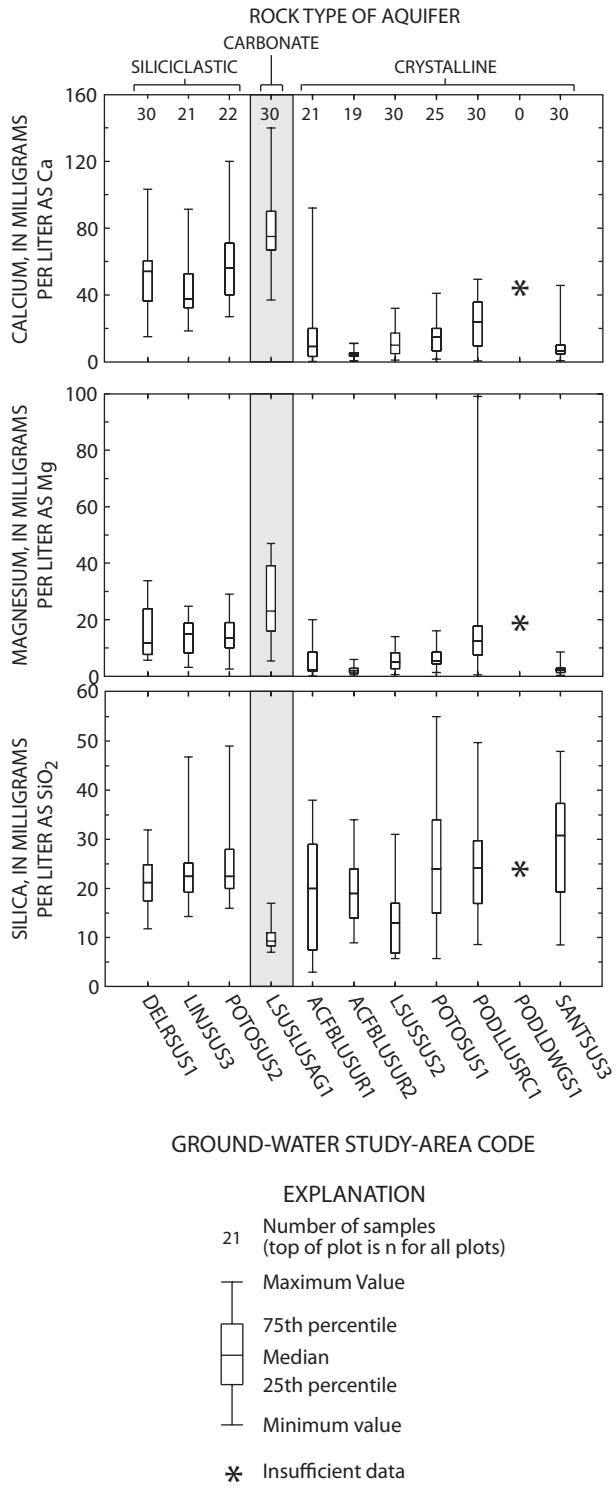

Figure 16. Summary of concentrations of calcium, magnesium, and silica for ground-water samples collected by the USGS NAWQA Program from ground-water study areas in the Piedmont Aquifer System, eastern United States. (Ground-water study-area codes are defined in table 2.)

Dissolved oxygen concentrations typically are in the range indicating well-oxygenated water. The presence of dissolved oxygen is important in relation to geochemical processes controlled by oxidation-reduction reactions. Iron is an example of a constituent controlled by oxidation-reduction reactions. In the presence of oxygen, iron precipitates, and in the absence of oxygen, iron is more likely to be dissolved. Other constituents also are controlled by these reactions. Some, like iron and manganese, are not specifically addressed in data analysis because they do not have a primary maximum contaminant level and are not considered to be a human-health threat. Concentrations of other constituents, such as nitrate and some of the organic compounds, also can be directly affected by oxidation-reduction processes; therefore, dissolved oxygen is an important explanatory variable in data analysis. For example, anoxic conditions and isolation from the atmosphere may increase the likelihood of denitrification, a process that transforms nitrate into nitrogen gas. Aquifers with characteristics that allow water to be rapidly transmitted from the land surface to the water table are likely to be well oxygenated and, there foe, less likely to have processes such as denitrification occurring. In parts of the carbonate-rock aquifers where conduit flow occurs, aeration and turbulence can maintain sufficient dissolved oxygen in the water, further decreasing the possibility of denitrification.

Major ion chemistry is another issue directly related to bedrock type. The concentrations of calcium and magnesium are greatest in the carbonate rocks, from dissolution of the calcite and dolomite that are the major minerals in limestone and dolomite, respectively. The concentrations of calcium and magnesium in the crystalline rocks are relatively low because of the lack of carbonate minerals in these rocks. The concentrations of calcium and magnesium in the siliciclastic rocks are between those concentrations in the crystalline rocks and those concentrations in the carbonate rocks. Conversely, the concentrations of silica are greatest in the siliciclastic-rock and crystalline-rock aquifers because of the presence of the silicate minerals in the rocks, and concentrations of silica are low in water from the carbonate-rock aquifers. Concentrations of iron and manganese were low; iron concentrations exceeded the Secondary Maximum Contaminant Level (SMCL) of 0.3 mg/L in 11 percent of the samples, and manganese exceeded the SMCL of 0.05 mg/L in 21 percent of the samples. A SMCL is a non-enforceable standard and typically is related to aesthetic issues such as taste, odor, or staining. The iron and manganese data sets had a skewed population; the median concentrations were much lower than the SMCLs. Iron was inversely correlated with dissolved oxygen. As previously stated, iron is highly sensitive to the oxidation-reduction reactions; therefore, the inverse relation seen between oxygen and iron is expected. Less than 1 percent of the samples had concentrations of sulfate that exceeded the SMCL of 250 m/L. Sulfate also is affected by oxidation-reduction reactions and had a negative correlation with dissolved oxygen. No samples had chloride concentrations that exceeded the SMCL of 250 mg/L, nor did any sample have concentrations of fluoride that exceeded the SMCL of 2 mg/L.

Statistical Methods Used to Analyze Water-Quality Data

Interpretation of the water-quality data from the PAS included use of statistical methods. These methods included comparisons of water quality among groupings (categorical comparison), comparison of water quality to continuous explanatory variables (correlation and linear regression), and comparison of water quality to explanatory variables using discrete categories (logistic regression). These methods were intended to illustrate the factors affecting water quality. Although some of these methods can be used to predict water quality in unsampled areas, those predictions are beyond the scope of this report.

Categorical Statistics

Interpretation of data with a continuous response variable and categorical explanatory variable was conducted using the Tukey's Test (Tukey, 1977). An example of this type of comparison would be determining differences in median nitrate concentration among lithologic groups. The purpose of this method is to test whether group medians differ and which groups differ from other groups. The alpha value used for these tests was 0.05, which means there is a 95-percent confidence that the differences among the groups are not due to random chance. The Tukey's Test assigns letters to each category on the basis of the statistical grouping to which that category belongs. The groups with the highest medians are assigned the letter "A," the second highest medians are assigned the letter "B," and groups are assigned subsequent letters based on descending medians. The Tukey's Test may result in a category being assigned more than one letter. For example, a category may belong to both statistical group "A" and statistical group "B" in a case where a category is not statistically different from the category above or below it, but the above and below categories are different from each other.

Continuous Explanatory Variable Statistics

In cases where there is a continuous explanatory variable and a continuous response variable, a Kendall's tau correlation or multiple linear regression was used. A continuous variable can have any value within a certain range. An example of this type of comparison is the comparison of the application rate of fertilizer (continuous explanatory variable) to the concentration of nitrate (continuous response variable). The most frequently used statistic was the Kendall's tau correlation (Helsel and Hirsch, 1992, p. 105). This method uses ranks of data to determine a monotonic relation between the explanatory variable and the response variable. The statistics produced by the Kendall's tau test are the Kendall's tau coefficient and the probability (or p-value). P-values of less than 0.05 indicate a 95-percent confidence level that a monotonic relation between the explanatory variable and the response variable exists. That is, an increase in the explanatory variable is correlated to an increase in the response variable. The values of Kendall's tau range from 0 to 1; larger values indicate a stronger relation. The sign of Kendall's tau is an indicator of whether the relation has a positive or negative slope.

Kendall's tau is effective in determining relations between a single continuous explanatory variable and a continuous response variable, but it does not account for the interaction among multiple explanatory variables. In cases where there are sufficient data and multiple explanatory variables, a multiple linear regression can be performed. This determines the linear relation between multiple explanatory variables and the response variable as determined by equation 1:

$$y = b_0 + b_1 x_1 + b_2 x_2 + \ldots b_i x_i + \Sigma \quad (1)$$

where b_0 is constant, x_1 is explanatory variable 1, b_1 is slope coefficient of x_1, x_2 is explanatory variable 2, b_2 is slope coefficient of x_2, x_i is explanatory variable i, b_i is slope coefficient of x_i and Σ is random error.

A model is developed to determine the solution for equation 1 that best fits the observed data. Those explanatory variables that are statistically significant (p-values less than 0.05) are included in the model. The implication is that only those variables that improve model fit are retained. The power of the model is indicated by the r-square result, which is the sum of squared residuals. Higher r-square values indicate a better fit between observed and predicted values.

Discrete Response Statistics

A discrete variable is one who's values are limited to specific categories, such as greater than or less than a detection limit or specified threshold. In cases where the response variable is discrete, logistic regression can be used to determine the probability of the response variable exceeding a threshold. An example of this would be testing whether increases in pesticide application rate cause an increased probability of that pesticide exceeding the detection limit. The probability of an event occurring is defined by equation 2:

$$p = \frac{e^{(b_0 + b_1 x_1 + b_2 x_2 + \ldots b_i x_i)}}{\left[1 + \left(e^{(b_0 + b_1 x_1 + b_2 x_2 + \ldots b_i x_i)}\right)\right]} \quad (2)$$

where b_0 is constant, x_1 is explanatory variable 1, b_1 is slope coefficient of x_1, x_2 is explanatory variable 2, b_2 is slope coefficient of x_2, x_i is explanatory variable i, b_i is slope coefficient of x_i (Helsel and Hirsch, 1992, p. 396). Analyzing the results of logistic regression is more complicated than analyzing the results of linear regression. Statistics that are important are 1) the overall significance of the model, 2) the value and probability value of explanatory variables, 3) the Hosmer-Lemeshow results, 4) the generalized r-square, 5) the maximum rescaled

r-square, 6) the percent concordance, and 7) the Pearson residuals.

The overall significance of the model, indicated by p-values less than 0.05, indicates that the model with explanatory variables is better at predicting the probability of an event occurring than an intercept-only model. The significance of the explanatory variables, indicated by p-values less than 0.05, indicates that a specific explanatory variable improves the model in its ability to predict the probability of an event occurring. The Hosmer-Lemeshow Goodness-of-Fit statistic (Hosmer and Lemeshow, 1989) tests whether or not the outcomes predicted by the model are significantly different than the outcomes from the original data. P-values of a Hosmer-Lemeshow test that are less than 0.05 indicate the model predictions and the data are significantly different; however, the model predictions should fit the data. Therefore, p-values less than 0.05 indicate a poor model fit. There is no r-square value that can be produced by the logistic regression model that is identical to the r-square value from linear regression; however, some substitutes for the r-square value have been calculated. The generalized r-square value (Cox and Snell, 1989) is based on maximizing the log-likelihood and is a generalized method of estimating an r-square value.The maximum-rescaled r-square value (Nagelkerke, 1991) is another method that approximates the linear-regression r-square. Although neither of these statistics can be interpreted as the percentage of variance explained by the model, they can be used as comparisons of one model to another.

The terms concordance and discordance also are used in describing results of logistic regression. These statistics are calculated by comparing every possible combination of data points where one event is equal to '1' and the other event is equal to '0.' If the predicted probability for the case with event equal to '1' is higher than the predicted probability for the case with the event equal to '0,' that pair is concordant. The opposite case would be discordant, and ties are also counted; however, concordance is the primary statistic used in this report.

The ability of the model to predict individual cases also can be evaluated by examination of the residuals. Raw residuals are calculated by the observed frequency minus the expected frequency. Pearson residuals are a similar statistic and represent the contribution of each observation to the Pearson Chi-square. Cases where the model predicts a low probability of an event occurring, but it occurs anyway, will have a high Pearson residual. Cases where the model predicts a high probability of an event occurring, but it does not occur, have a large negative Pearson residual. Observing the cases with the highest and lowest Pearson residuals can illustrate the unique conditions where the model does not do a good job of predicting the event.

Occurrence and Distribution of Selected Contaminants in the Piedmont Aquifers

Sampling by the NAWQA Program in the PAS covers a broad geographic area, three types of bedrock aquifers, and several land-use settings. This, in conjunction with the numerous types of samples collected at most sites, provides an opportunity to examine the occurrence and distribution of a broad range of contaminants. In addition to evaluating the occurrence and distribution, factors affecting the occurrence and distribution are examined. Some of the contaminants are related to human activities (anthropogenic) and others occur naturally. Analysis will focus on those contaminants that were measured at nearly every site and have potentially adverse effects on human health: nutrients (predominantly nitrate - anthropogenic), pesticides (anthropogenic), VOCs (anthropogenic), and radon (natural). The U.S. Environmental Protection Agency (USEPA) has established Maximum Contaminant Levels (MCLs) for public drinking water for many of these contaminants. The majority of the wells sampled for this study are not public-supply wells and, therefore, are not subject to the MCL; however, the MCL or other established health standards are referred to for comparison purposes.

Nitrate in Ground Water

Applications of nitrogen fertilizer in the United States have increased by a factor of 20 in the years from 1945 to 1985 (Puckett, 1994). Atmospheric deposition of nitrogen and the number of septic systems have increased during this time period as well. Nitrate is soluble in water and therefore can enter the ground water and become a health concern. The USEPA has established the MCL for nitrate at 10 mg/L as nitrogen. The main health risk from nitrate in drinking water is a condition called methemoglobinemia, which can be fatal in infants. Many rural domestic water supplies receive no treatment prior to use. A national study of nitrate in ground water showed that 15 percent of wells sampled in major aquifers exceeded the USEPA MCL of 10 mg/L (Nolan and Stoner, 2000). Samples were collected for nutrient analysis in 10 studies in the PAS. The results of this sampling were analyzed to determine spatial patterns and transport mechanisms that affect nitrate concentrations in the PAS.

Samples were collected for nutrient analysis at 241 wells and 19 springs in the PAS. Nutrient samples were analyzed by the USGS National Water-Quality Laboratory (NWQL) for organic nitrogen, ammonia, ammonia plus organic nitrogen, nitrite, nitrate plus nitrite, phosphorus, and orthophosphate. Concentrations of phosphorus, nitrite, ammonia, and organic nitrogen were low. The maximum concentrations of phosphorus and orthophosphate were 0.25 and 0.27 mg/L as phosphorus, respectively. The maximum concentration of ammonia plus organic nitrogen was 2.8 mg/L, and only 14 of the 260 samples exceeded 0.2 mg/L. The maximum concentration of nitrite was 0.38 mg/L, and only 17 samples had concentrations greater than 0.1 mg/L as nitrogen. The predominant form of nitrogen detected in water from wells was nitrate. The laboratory reports a concentration of nitrate plus nitrite, but because nitrite concentrations were so low, these results were considered to be equivalent to nitrate. The concentrations of nitrate plus nitrite

(hereafter referred to as nitrate) in water from wells in the PAS ranged from below the detection limit of 0.05 mg/L to 25 mg/L as nitrogen. Only 32 of the 260 samples had concentrations below the detection limit. Concentrations of nitrate exceeded the USEPA MCL of 10 mg/L in 29 samples. Because nitrate was detected in ground-water samples across a broad range of aquifer types and environmental settings, the approach to analyzing these data was to try to determine the relations between the intensity of potential nitrogen sources, the susceptibility of the aquifer to infiltration of contaminants, and the resulting concentrations of nitrate in ground water.

Nitrogen Sources

Nitrogen is present in the environment in many forms. Typically, nitrogen is not found in elevated concentrations in ground water in the environment without an anthropogenic source. These sources can include atmospheric deposition, human sewage, animal waste, and chemical fertilizer. Understanding the sources of nitrogen and the nitrogen cycle is important when trying to identify causes of elevated nitrogen or nitrate in ground water. For example, the manure applied to cropland as a fertilizer may have a concentration of nitrogen similar to that of human-waste effluent from a septic system. However, the manure is subject to many processes such as plant uptake, volatilization, and denitrification that may attenuate the nitrogen concentrations prior to entering the ground-water system, whereas septic effluent may enter the ground-water system directly without being subject to many of these processes. The potential locations of anthropogenic sources can be inferred from land use, and land use typically is used as a general indicator of nitrogen sources. In addition to land use, data on specific sources are available as well. These data are all compiled for the 1,640-ft radius around the well. Data are available to estimate the spatial distribution of nitrogen from atmospheric deposition (Hitt, 2005b). Fertilizer-sales data have been used to infer application rates of fertilizer. Typically, fertilizer usage is estimated for agricultural rather than residential use, but residential use also has been estimated (Hitt, 2005c). The amount of manure generated by animals in a given area commonly is used as an indicator of potential application of manure for fertilizer (Hitt, 2005c). The amount of nitrogen from septic systems was estimated using equation 3:

$$N_s = Ce \times Ve \times n \quad (3)$$

where N_s is the mass of nitrogen input from septic effluent, Ce is concentration of nitrogen in septic effluent (85 mg/L; Miller, 1980), Ve is the volume of septic effluent per person per day (170 L/day; Miller, 1980), and n is the number of people using septic systems in the areal extent of the zone of contribution to the well [assuming four persons per household and using septic-system density from Hitt (2005a)]. A summary of the sources of nitrogen in the 10 study areas where nitrate samples were analyzed has been compiled in table 7. No nitrate analyses are available for the podldwgs1 study.

Table 7. Sources of nitrogen in NAWQA ground-water study areas of the Piedmont Aquifer System.

Ground-water study-area code[1]	Median input from 1,640-ft radius around wells in each study Nitrogen, in kilograms per square kilometer per year						Median nitrate concentration
	Septic systems[2]	Atmospheric deposition[3]	Non-farm fertilizer use[4]	Farm-fertilizer use[4]	Animal manure[4]	Total nitrogen input all sources[5]	
acfblusur1	89	493	0	0	0	465	1.6
acfblusur2	236	503	0	0	0	586	1.3
delrsus1	251	483	1,081	1,377	837	3,505	3.1
linjsus3	260	485	957	1,219	447	2,889	1.6
lsuslusag1	318	639	3,244	4,133	20,188	23,152	11.0
lsussus2	253	660	2,206	2,810	2,512	7,407	6.6
podllusrc1	250	653	301	383	259	1,681	1.0
potosus1	146	669	1,424	1,814	1,247	5,235	1.4
potosus2	122	663	1,448	1,844	1,521	4,996	.9
santsus3	161	475	377	481	687	1,834	.7

[1]Ground-water study-area codes are defined in table 2.

[2]Calculated from eq. 3 and population using septic tanks for sewage disposal from Hitt (2005a).

[3]Data from Hitt (2005b).

[4]Data from Hitt (2005c).

[5]Totals are medians from study area and do not sum across table.

Distribution of Nitrate Concentrations

In addition to the sources of nitrogen, aquifer characteristics also affect the potential for detecting elevated concentrations of nitrate in ground water. These characteristics include aquifer permeability and organic content of aquifer materials. Aquifers with low permeability, or permeability that decreases with depth, will tend to have ground water that is older. In many cases, the traveltime from the land surface to the well allows denitrification to occur (Lindsey and others, 2003). The distance from the land surface to the water table can affect fate and transport of nitrate as well. Concentrations of nitrate were highest in the LSUS study unit (fig. 17), which is the most highly agricultural area. Urban areas in the ACFB study unit had low concentrations of nitrate, as did the SANT study unit, which is the most heavily forested area (table 6, fig. 18). Those areas of the LINJ, DELR, and POTO that had mixed land uses had a range of nitrate concentrations from very low to high (fig. 19).

Initial analysis of nitrate concentrations in ground water was done using categorical comparisons among 10 study areas. In 8 of the 10 areas, median concentrations of nitrate were less than 3 mg/L, the crystalline-rock aquifers of the LSUS (lsussus2) had a median nitrate concentration of 7 mg/L, and the carbonate-rock aquifers of the LSUS (lsuslusag1) had a median nitrate concentration of 11 mg/L (fig. 19). Of the 29 samples that exceeded the USEPA MCL of 10 mg/L, 18 were in the lsuslusag1 study, 9 were in the lsussus2 study, 1 was in the podllusrc1 study, and 1 was in the santsus3 study (fig. 18). A Tukey's Test indicated three groups of nitrate concentrations were significantly different at a 95-percent confidence interval (fig. 17). The highest nitrate concentration group was lsuslusag1, the second highest was lsussus2, and all the remaining study areas were in the third group. These concentrations are a result of both the sources of nitrogen and the aquifer characteristics. A comparison of fig. 17 to table 7 illustrates the areas with the largest nitrogen inputs had the highest median nitrate concentrations; however, the susceptibility of the aquifers to contamination is a factor also. The transmission of contaminants into and through carbonate-rock aquifers has been documented; however, because of the lack of comparable study types (carbonate, non-agricultural; non-carbonate agricultural, table 6) this study does not have the data to determine whether aquifer vulnerability or land use is the cause of the high nitrate concentrations.

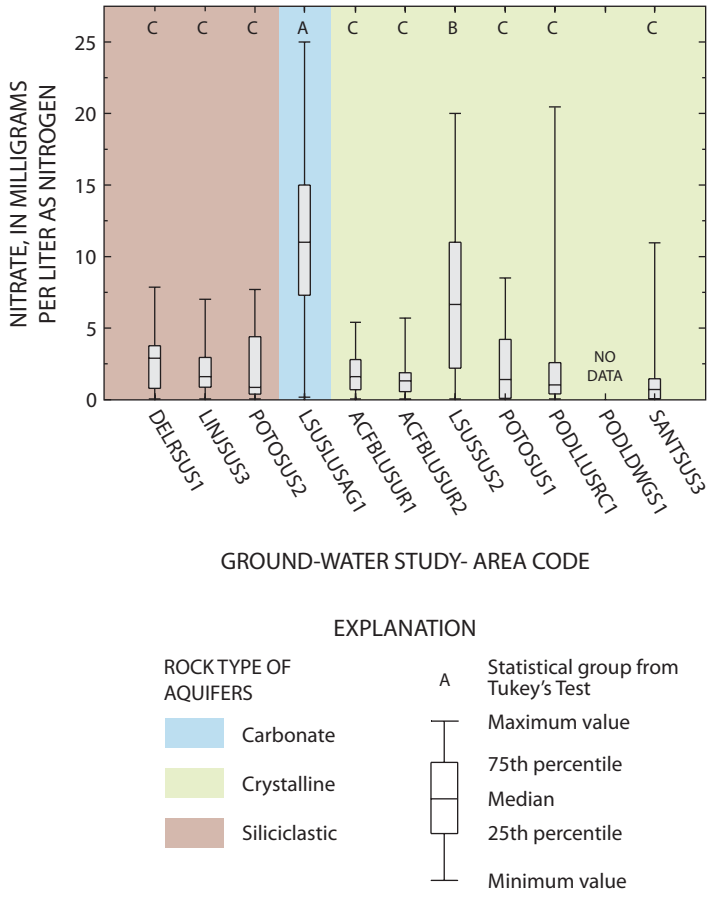

Figure 17. Distribution of concentrations of nitrate in ground water for NAWQA studies in the Piedmont Aquifer System, eastern United States. (Ground-water study-area codes are defined in table 2.)

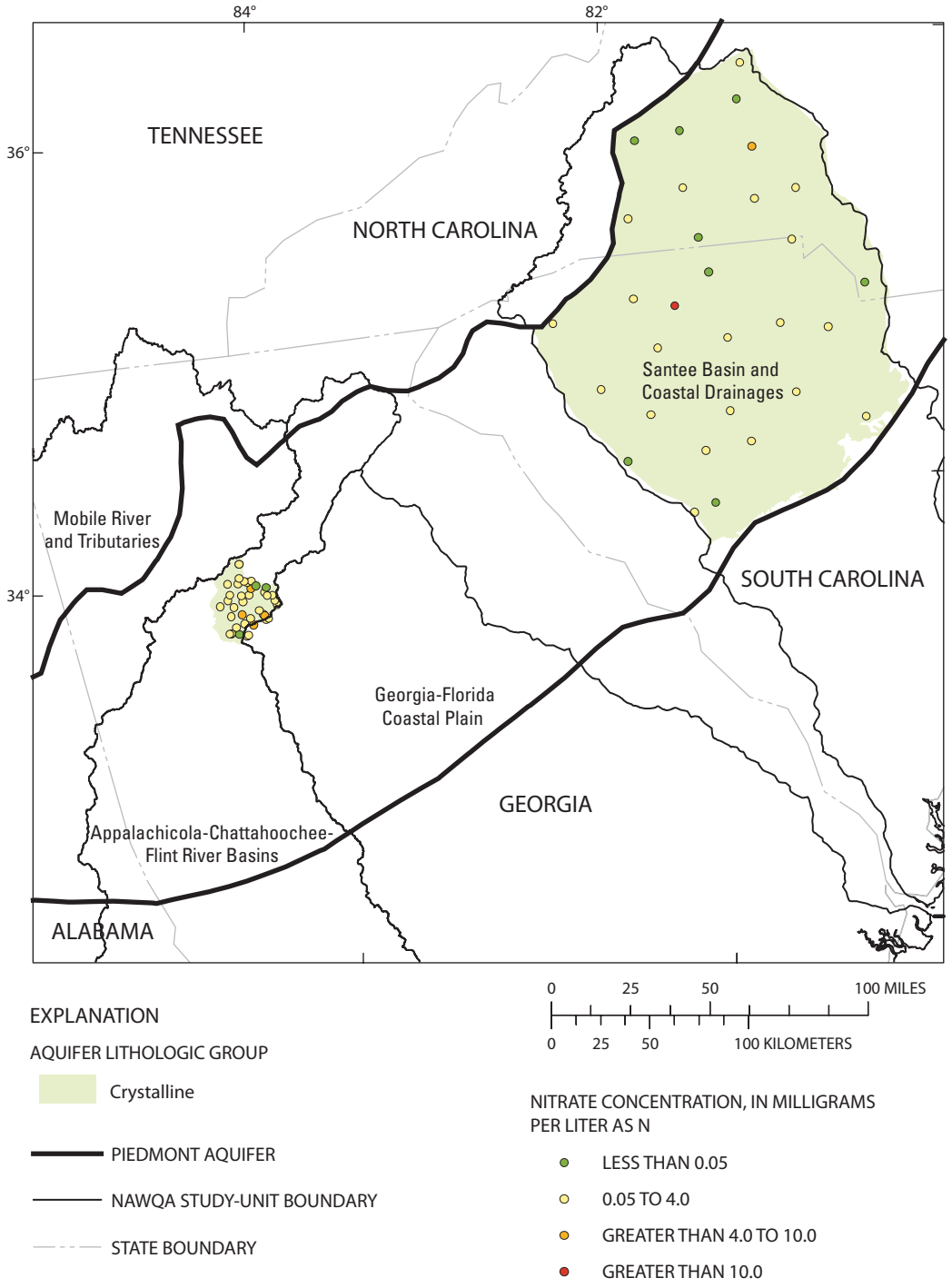

Figure 18. Concentrations of nitrate in ground-water samples from wells in the southern area of the Piedmont Aquifer System, eastern United States.

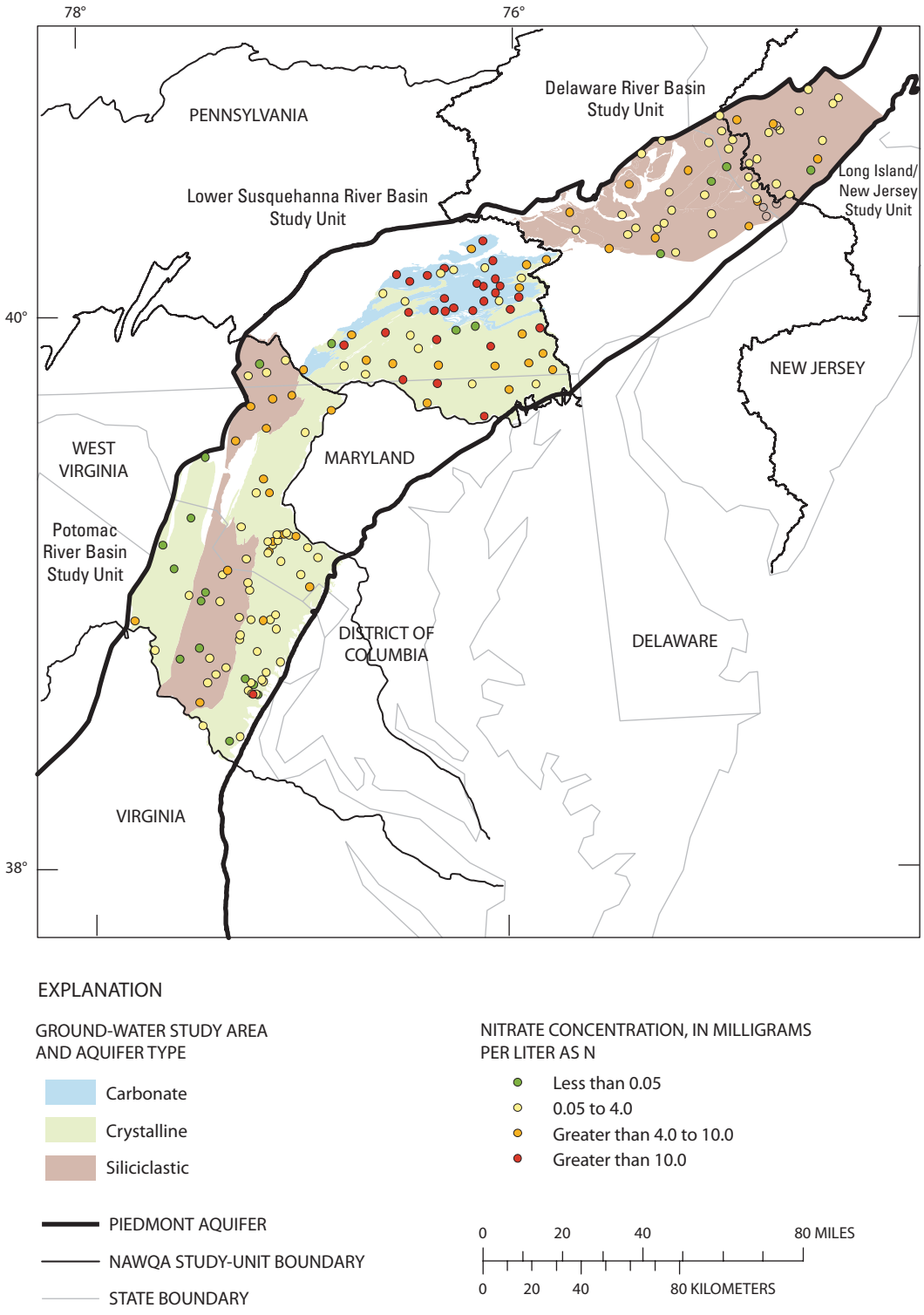

Figure 19. Concentrations of nitrate in ground-water samples from wells in the northern area of the Piedmont Aquifer System, eastern United States.

Factors Affecting Nitrate Concentrations

In order to determine the factors affecting nitrate concentrations for the areas studied, several statistical techniques were used. For categorical explanatory variables, tests such as the Tukey's test were conducted to determine statistical differences among categories. Then, individual correlations between continuous nitrate concentration and various continuous explanatory variables were determined using a Kendall's tau correlation. Explanatory variables included factors potentially related to nitrogen sources such as population density, land use, and nitrogen inputs. Other explanatory variables included transport variables such as soil hydrologic characteristics, aquifer type, permeability type, and well-construction characteristics. Characteristics relating to the well only (such as well-construction information) are summarized for individual wells and all other characteristics are summarized for an area within a 1,640-ft radius of the well. To determine the influence of the explanatory variables within each aquifer type, all correlations were first conducted for the entire data set, then repeated for each aquifer type.

Aquifer type is a categorical variable, therefore a nonparametric Tukey's test was conducted to determine differences among the three categories (carbonate, crystalline, and siliciclastic). This test indicated the carbonate rocks had a statistically significant higher median nitrate concentration than the other two bedrock types ($p < 0.0001$). When the samples from the carbonate-rock aquifer were removed, differences in median nitrate concentration between the crystalline- and siliciclastic-rock aquifers were not statistically significant. The test also was conducted comparing the type of permeability (porous media, fracture flow, and fracture/conduit flow) to nitrate concentration. The studies in the unconsolidated saprolite aquifer (acfblusur1 and acfblusur2) were designated as porous-media permeability, and the carbonate-rock aquifers study (lsuslusag1) was designated as fracture/conduit-flow permeability. Aquifers in all other areas were considered to have fracture-flow permeability. The category of fracture/conduit flow (carbonate rocks) had a statistically significant higher median nitrate concentration than the other two categories ($p < 0.0001$). The test was also repeated without the fracture/conduit category, and there were still no statistically significant differences between fracture-flow and porous-medium permeability types. It is difficult to draw conclusions about the effect of aquifer type and permeability type on nitrate concentration from this data set, though, because the only samples in carbonate rocks were from an agricultural land-use study and had inputs of nitrogen that were an order of magnitude higher than most of the other areas and the only studies in the unconsolidated saprolite aquifer were urban land-use studies that had inputs of nitrogen that were an order of magnitude lower than the other studies (table 7).

The results of the correlations between continuous explanatory variables and nitrate concentration are shown in table 8. All correlations that had at least one significant result are listed in the table. Correlations between nitrate and population density and the natural log of population density were not significant for any of the categories tested; therefore, the correlations are not included on table 8. The percentage of agricultural land use as well as hay and pasture around a well had statistically significant positive correlations to nitrate concentration for the entire data set, the crystalline-rock aquifers, and the siliciclastic-rock aquifers. The percentage of row crops was significantly correlated to nitrate concentration for the entire data set as well as the crystalline-rock aquifers. The fact that more significant correlations were determined for hay and pasture than for row crops is counterintuitive because the input of nitrogen to hay and pasture land is typically lower than that for row crops. This may be related to crop rotation where hay and row crop land use vary annually. It may also be because row crop and hay and pasture categories are significantly related to each other (Kendall's tau correlation coefficient = 0.57; $p < 0.0001$), indicating a good possibility that hay and pasture and row crop are surrogates for each other, and the general category of agricultural land use is a better category to use. The lack of correlation between agricultural land use and nitrate concentration within the carbonate-rock aquifers is likely because of the fact that the carbonate study targeted agricultural land (the median of agricultural land use in the 1,640-ft radius around the wells is 97 percent). It is the lack of variation in percentage of agricultural land use for the carbonate aquifer that leads to the poor correlation between land use and nitrate concentration in this area.

The statistical tests illustrated a significant positive correlation between nitrate concentration and total nitrogen sources for the entire data set, the crystalline-rock aquifers and the siliciclastic-rock aquifers. The correlation pattern was the same when comparing nitrate concentration to nitrogen from chemical fertilizer, nitrogen from manure, and nitrogen from atmospheric deposition (for all but the siliciclastic-rock aquifers). Lack of correlations between nitrogen sources and nitrate concentrations within the carbonate-rock aquifers are because of the uniformly high nitrogen input for all wells in that data set that was an order of magnitude higher than for the other study areas. The largest correlation coefficient between factors representing potential nitrogen sources and nitrate concentration for the entire data set was for the input of chemical fertilizer.

The correlations between nitrate and dissolved oxygen concentration had statistically significant positive correlation coefficients for the entire data set and within each of the three aquifer types (all correlations are positive unless otherwise noted). Dissolved oxygen can be a surrogate for several factors that relate to nitrate concentrations at an individual well. These factors, such as the organic content of aquifer materials and potential denitrification, may vary on a very small scale that is not mappable. Therefore, dissolved oxygen would have to be sampled in individual wells, is not easily amenable to extrapolation beyond the sampling point, and is not useful in predicting nitrate concentrations on a regional scale.

Characteristics of well construction were compared to nitrate concentrations. Well depth and casing length were not statistically significant explanatory variables for any of the categories and, therefore, are not shown on table 8. A weak but sta-

Table 8. Correlations between nitrogen concentrations and explanatory variables in water from wells in the Piedmont Aquifer System by use of Kendall's tau correlation.

[n, number of samples; Total nitrogen, nitrogen inputs in 1,640-ft radius around the well from atmospheric deposition, manure, and fertilizer; Agricultural land use, percentage of row crop and hay and pasture in 1,640 -ft radius around well; NS, No statistically significant correlation at an alpha value of 0.05; <, less than]

	Kendall's tau Correlation Coefficient Probability Values (p=)			
	All Data n = 259	**Crystalline-rock aquifers n = 155**	**Carbonate-rock aquifers n = 30**	**Siliciclastic-rock aquifers n = 74**
Land use[1]				
Agricultural land use	0.336 <.0001	0.244 <.0001	NS	0.169 .0347
Row crop	.277 <.0001	.200 .0005	NS	NS
Hay/pasture	.279 <.0001	.249 <.0001	NS	.170 .0343
Potential contaminant sources[2]				
Total nitrogen	.350 <.0001	.253 <.0001	NS	.157 .0474
Nitrogen from fertilizer	.349 <.0001	.291 <.0001	NS	.167 .0348
Nitrogen from animal manure	.303 <.0001	.178 .0014	NS	.156 .0479
Nitrogen from atmospheric deposition	.154 .0002	.164 .0027	NS	NS
Physical or chemical data collected at the time of sampling				
Dissolved oxygen concentration	.310 <.0001	.335 <.0001	.326 .0128	.323 <.0001
Hydrogeology and soils [3]				
Water level (ft below land surface)	.116 .0096	NS	NS	NS
Percentage soil in hydrologic group A	.215 <.0001	.384 <.0001	NS	NS
Percentage soil in hydrologic group B	NS	NS	NS	.270 .0010
Percentage well drained soils (group A + group B)	NS	NS	NS	.33 .0036
Percentage organic matter	NS	NS	NS	-.164 .045
Percentage clay	-.137 .0014	-.204 .0003	NS	-.281 .0079
Percentage silt	.173 <.0001	.163 .0039	NS	-.218 .0079
Percentage sand	NS	NS	NS	.291 .0004

[1]Data in percent for 1,640-ft radius around well from Vogelmann and others (1998a, 1998b).

[2]Nitrogen in kilograms for 1,640-ft radius around well from Hitt (2005b, 2005c).

[3]Average percent soil composition for 1,640-ft radius around well from U.S. Department of Agriculture (2003).

tistically significant positive correlation existed between nitrate concentration and water level; deeper water levels were associated with higher nitrate concentrations. This is similar to findings of Hitt and Nolan (2005), who indicated that water levels close to the land surface have a low likelihood of nitrate contamination because waterlogged soils have a high potential for denitrification.

Soil characteristics also were compared to nitrate concentrations (table 8) to determine if presence of high permeability soils is related to higher nitrate concentrations. The percentage of soils in hydrologic group 'A' (the highest permeability soils; U.S. Department of Agriculture, 2003) had a significant positive correlation to nitrate concentration for the entire data set as well as the crystalline-rock aquifers. The percentage of soils in hydrologic group 'B' (the second highest permeability soils) was significantly correlated to nitrate concentration for the siliciclastic-rock aquifers. There were essentially no soils with hydrologic group 'A' in the siliciclastic-rock aquifers, which explains the almost identical correlations for nitrate concentrations to the percentage of well-drained soils (the combination of soils in hydrologic group 'A' and hydrologic group 'B'). The only area where a significant correlation existed between the percentage of organic matter and nitrate concentration was in the siliciclastic-rock aquifers. This was a negative correlation (higher organic matter was associated with lower nitrate concentration). This could be because of the fact that this is the only area in which organic matter in the soil horizon had values high enough to affect nitrate concentrations. Although organic matter is low in all the aquifer types, the highest median value (0.7 percent) and the highest maximum value (0.9 percent) were in the siliciclastic-rock aquifers. Percentage clay has a statistically significant negative correlation to nitrate concentration in all areas except for the carbonate-rock aquifers. The negative correlation is related to the fact that clay is associated with low permeability and thus may decrease leaching of nitrate through the unsaturated zone. Percentage sand has a positive correlation to nitrate concentration for the siliciclastic-rock aquifers and may indicate that the higher permeability of sands allows more nitrate to leach into the ground water. The percentage of silt is negatively correlated to nitrate concentration in the siliciclastic-rock aquifers but is positively correlated to nitrate concentration in the crystalline-rock aquifers. Without more detailed information on the entire distribution of particle sizes in soil horizons in those two aquifers, it would be speculative to draw conclusions about the relation between percentage silt and nitrate concentration.

One of the difficulties in determining the importance of individual factors affecting water quality is the interrelation between susceptibility factors (such as soil permeability) and source factors (such as land use). In order to evaluate these effects simultaneously, a multiple linear regression was conducted using several variables at once. All variables that had statistically significant correlations (table 8) were evaluated. When using all data, the regression showed that a combination of source factors (percentage of agricultural land use and total nitrogen from manure) and transport factors (dissolved oxygen) were statistically significant variables at a 95-percent confidence interval (table 9). The overall p-value for the test was <0.0001 and the r-square value was 0.49. In part, the regression is constrained by the fact that the single carbonate study area has high values for all the significant variables. The carbonate-rock aquifers have median nitrate concentrations that are significantly higher (fig. 17) than concentrations in all the other categories yet make up a small percentage of the overall area of the PAS. This area also has the highest dissolved oxygen concentrations, manure input, and percentage of agricultural land use. To determine how much this affects the regression, the model was run without the samples from the carbonate-rock aquifers. The regression had similar results, with the exception that the r-square value was only 0.28. These results provide insight to the factors that affect nitrate concentrations but do not provide enough statistical power to predict concentrations in other areas where samples were collected or to extrapolate the results to a larger area than the areas sampled. To do this would require additional samples in ground-water study areas with a broad range of sources and aquifer characteristics that result in a range of nitrate concentrations, and there is no certainty that this would produce a reliable predictive model.

Another method to analyze the factors affecting nitrate concentration is to use logistic regression. Logistic regression is used to predict the probability of the modeled response being in a category, such as exceeding a threshold value. The probability of that event occurring is defined by equation 2.

A logistic regression model was built using a threshold concentration of 4 mg/L. That threshold was selected because it was near the median value for the data set, as well as being a concentration associated with human-health effects (Ward and others, 1996). In addition, national NAWQA studies of nitrate in ground water have used the threshold of 4 mg/L (Hitt and Nolan, 2005; Nolan, 2001). The logistic-regression model tested the same variables used for the linear-regression model. A backward elimination procedure was used to subtract variables from the model until the number of significant variables

Table 9. Summary of statistics for a linear regression model for nitrate concentration in the Piedmont Aquifer System, eastern United States.

[<, less than]

	Results for variable		
	Statistically significant variables	**Parameter estimate**	**Probability (p-value)**
Model	y-intercept	2.75	0.579
	Dissolved oxygen	.343	<.0001
	Total nitrogen from manure	.0005	<.0001
	Percent agricultural land use	.026	.05

was maximized. Significant variables were those that had a Wald Chi-Square probability of less than 0.05.

Two models were constructed for this exercise. Model one was constructed to include all available variables and model two was constructed using only spatial data that could be determined without field measurements so that it would be possible to extrapolate results to unsampled areas. Variables such as well-construction characteristics and dissolved oxygen were not included in model 2.

The overall fit for model 1 was statistically significant with a Wald Chi-Square probability value of < 0.0001. Those variables that were significant in the optimal logistic regression model (table 10) were dissolved oxygen concentration, total nitrogen input, and percentage of agricultural land use. Because the units of the regression differ among categories, the standardized regression coefficient is shown (table 10). This statistic allows comparisons among variables in the model in common units (Menard, 2002) and indicates that variation in dissolved oxygen is the most significant variable in model 1. The logistic regression model was assessed by the concordance, the Hosmer-Lemeshow Test, and the generalized and maximum-rescaled r-square values. The comparison of observed and predicted responses indicated 87 percent of the cases were predicted correctly (concordant) and 13 percent of the cases were incorrectly predicted (discordant). The Hosmer-Lemeshow test divides the data into deciles and compares the expected and observed outcomes in each decile. The Hosmer-Lemeshow p-value was 0.79, which indicates good model fit (p-values of less than 0.05 would indicate a poor model fit). The generalized r-square value was 0.36, and the maximum-rescaled r-square value was 0.51. These r-square values are not identical to r-square values for linear regression but do provide a measure of how well the model fits the data.

The overall fit for model 2 was statistically significant with Wald Chi-Square probability value of < 0.0001 (table 10). The variables that were significant in model 2 were percentage silt, total nitrogen input, percentage agricultural land use, percentage sand, and percentage organic matter. Percentage silt and total nitrogen input had the highest standardized coefficients, indicating these two variables are the most significant in the model. The relation between percentage organic matter and probability of nitrate exceeding 4 mg/L was an inverse relation. The comparison of observed and predicted responses indicated that 85 percent of the cases were predicted correctly (concordant) and 15 percent of the cases were incorrectly predicted (discordant). The Hosmer-Lemeshow had a p-value of 0.59. The generalized r-square value was 0.32, and the maximum-rescaled r-square value was 0.46.

Further evaluation of models was attempted to determine the strengths and weaknesses of the predictions. The Pearson residuals were calculated for both models. Pearson residuals are high when the model predicts a small probability of exceeding the selected threshold at a given location, but the sample at that

Table 10. Summary of statistics for two logistic regression models assessing the probability that nitrate exceeds 4 milligrams per liter in the Piedmont Aquifer System, eastern United States.

[--, no data; <, less than]

	Results for variable				Results for model			
	Statistically significant variables	Parameter estimate	Probability (p-value)	Standardized coefficient	Percent concordant	Hosmer Lemeshow probability[1]	Generalized r-square[2]	Maximum rescaled r-square[3]
Model 1	intercept	-4.33	<0.0001	--	87.0	0.79	0.36	0.51
	Dissolved oxygen	.29	<.0001	0.511				
	Total nitrogen input	.0001	.0027	.445				
	Percentage agricultural land use	.02	.0030	.440				
Model 2	intercept	-7.5384	.0006	--	84.7	.59	.32	.46
	Percentage silt	.0962	.0029	.540				
	Total nitrogen input	.0002	.0029	.530				
	Percentage agricultural land use	.0195	.0149	.389				
	Percentage sand	.0862	.0194	.364				
	Percentage organic matter	-4.0212	.0239	-.369				

[1]Hosmer and Lemeshow, 1989.

[2]Cox and Snell, 1989.

[3]Nagelkerke, 1991.

point exceeds that threshold. Large negative Pearson residuals are found when the model predicts a high probability of exceeding a threshold, but the threshold is not exceeded. The analysis of the Pearson residuals indicated two cases where predictions were systematically weak. One situation was where a well with a high percentage of agricultural land use and a high nitrogen input was predicted to exceed the threshold of 4 mg/L but did not. In all four of cases where this situation existed, the dissolved oxygen concentrations were low (less than 1 mg/L). Although dissolved oxygen is accounted for in the model, it may reach a threshold where it becomes the controlling factor regardless of land use and nitrogen input. The other cases with high Pearson residuals were situations where agricultural land use was absent and nitrogen inputs were minimal, but the threshold of 4 mg/L was exceeded. These cases were all in urban areas and likely represent an undocumented nitrogen source, such as a leaking sewer line or over-application of lawn fertilizers. Other possible explanations for the inability of the model to correctly predict the probability of nitrate exceeding 4 mg/L would be complexities of the aquifer that are not captured by the spatial data sets, such as anisotropy. The true contributing area may not coincide with the 1,640-ft radius used to obtain the spatial data used for most of the explanatory variables.

Both the linear and logistic regression models were assessed for multi-colinearity. All the significant variables in both models (dissolved oxygen, nitrogen load, and percentage of agricultural land use) were assessed for multi-colinearity. The variance inflation factor (VIF) was calculated for each of these variables using a linear regression. The maximum VIF for these variables was for nitrogen load and percentage of agricultural land use, with a value of 2.25. This is below the threshold of 2.5 that indicates that multi-colinearity may affect the variance of the parameter estimates.

The results of the analysis of nitrate data in the PAS indicated a statistically significant relation between nitrate concentration and the explanatory variables of percentage of agricultural land use, nitrogen inputs, type of permeability, and dissolved oxygen. These factors are statistically significant, but lack of data precluded model validation. Model validation was attempted but was not successful. The data set was separated into a calibration data set and a validation data set (85 and 15 percent, respectively), but the model resulting from the validation data was completely different than the model from the calibration data set. This indicates the number of data points was insufficient to validate the model. In other studies, factors such as soil type, aquifer permeability, recharge rate, depth to water, well depth, and depth to open interval have been determined to be factors that affect nitrate concentration. It is likely that, within the PAS, the range of some of these factors is not sufficient to make them statistically significant variables. In other cases, there may be a range among the study areas, but not within the study areas. For example, the urban land-use studies tended to have very shallow wells, and the agricultural land-use study had a narrow range of well depths near 200 ft. This characteristic of the data set made it difficult to discern differences caused by some of these variables.

Maps predicting nitrate concentration on the basis of the linear regression or the probability of exceeding 4 mg/L on the basis of logistic regression will not be presented for several reasons. For both linear regression and logistic regression, r-square values are less than 0.5. Also, dissolved oxygen concentration in individual wells was a significant explanatory variable in both models, and spatial data to allow mapping dissolved oxygen concentration are not available to allow a broad extrapolation of these results. Additionally, because samples are not spatially distributed, the water-quality data used to create these models were not necessarily representative of the entire PAS. Therefore, the findings about the factors affecting nitrate concentrations are presented to enhance the understanding of the occurrence of nitrate in ground water. Further study and additional data would be needed to build a model that would allow predictions of nitrate concentrations or a model that would predict the probability of nitrate exceeding a threshold value.

Pesticides in Ground Water

Applications of pesticides in the United States increased from 617 million pounds of active ingredient in 1964 to a peak usage of 1,144 million pounds in 1979 and decreased to 888 million pounds in 2001 (Kiely and others, 2004). Agricultural uses account for the majority of pesticides applied in the United States, increasing from an estimated 366 million pounds in 1964 (59 percent of total), peaking at 843 million pounds in 1979 (74 percent total), and decreasing to 675 million pounds in 2001 (76 percent of total) (Kiely and others, 2004). Several of the older pesticides, such as DDT and dieldrin, are classified as persistent organic pollutants (POPs) because they breakdown relatively slowly in the environment and therefore may be detected in the environment years after their use has ceased (Jorgenson, 2001). Other pesticides, such as acetochlor or metolachlor, are relatively soluble in water, which may help facilitate their transport to aquifers (Barbash and Resek, 1996). Potential health effects from exposure to pesticides include damage to the nervous system, organ damage, reproductive problems, or an increased risk of cancer (U.S. Environmental Protection Agency, 2003). The USEPA has established MCLs for relatively few of the pesticides currently used in the United States (U.S. Environmental Protection Agency, 2003), although several other pesticides are listed on the contaminant candidate list for possible future regulation (U.S. Environmental Protection Agency, 2005). Pesticide degradates (breakdown products of pesticide-active ingredients resulting from biological, physical, or chemical processes) generally are not regulated by the USEPA but may have similar acute and chronic toxicity as their parent compounds (Kolpin and others, 1998).

A national study of pesticides in ground water showed at least one pesticide was in more than one-half of the shallow wells sampled in agricultural or urban areas, and many of those samples with detectable pesticides contained two or more pesticides (Fuhrer and others, 1999). Although pesticide concentrations in ground-water samples were rarely above drinking-water standards or guidelines, those guidelines do not account for the risk from synergistic effects from mixtures of multiple pesticides or degradates (Barbash and others, 1999). Another study of pesticides in ground water in Iowa found that degradates were detected in 75 percent of the wells sampled and that degradates constituted from 60 to over 99 percent of the total concentration measured for a given herbicide (Kolpin and others, 1998).

Pesticide Sources

Most pesticides are man-made chemicals and are not found in nature. Therefore, the presence of pesticides and their degradates in the environment is a direct result of human activity. Agricultural application of pesticides accounted for 76 percent of the total pesticide usage in the United States in 2001, the industrial/commercial/government and home/garden markets accounted for 12.5 and 11.5 percent, respectively (Kiely and others, 2004). Estimates of agricultural use of pesticides are available at the county level, but reliable estimates of non-agricultural pesticide use at the county level are nonexistent. This lack of data on non-agricultural use of pesticides makes data analysis difficult, especially in urban areas where the main application of certain pesticides (such as some of the insecticides) is thought to take place. Of the six pesticides (atrazine, simazine, alachlor, metolachlor, prometon, and dieldrin, plus the atrazine degradate—desethyl atrazine) chosen for statistical analysis, use estimates for the six NAWQA study units in the PAS where pesticide samples were collected are only available for alachlor, atrazine, metolachlor, and simazine, and only for agricultural uses at the county level (table 11).

Distribution of Pesticide Detections

Ground-water samples were collected for pesticide analysis from 251 wells and 19 springs in the PAS by NAWQA studies from 1993 to 2001. A single ground-water sample was analyzed from each site for dissolved pesticides by the USGS NWQL (Zaugg and others, 1995) for up to 44 pesticides and 3 degradates (table 12). Some compounds were added to the analysis during the study. The results of this sampling were analyzed to determine spatial patterns and factors that affect pesticide transport to the aquifers using Kendall's tau correlations and logistic regression.The herbicide acetochlor was not analyzed in 1993 and 1994; therefore, the ground-water studies lsuslusag1, lsussus2, potosus1, and potosus2 (92 samples in all) were not analyzed for acetochlor. The compounds propachlor, butylate, cyanazine, alpha-HCH, p,p'-DDE, parathion, ethalfluralin, terbacil, linuron, EPTC, pebulate, molinate, ethoprop, carbofuran, disulfoton, triallate, propanil, thiobencarb, and propargite were not analyzed in the podldwgs1 study.

The detection limit is not the same for each compound, and because of analytical changes during the study, detection limits vary over time for a single compound. Pesticide data can be either censored to the highest detection limit for all pesticides (referred to as a common censoring limit) or censored to the highest detection limit reported for each individual pesticide (referred to as an individual censoring limit). The term censoring does not imply that data are removed from the data set; rather, it indicates that any data between the highest and lowest detection limits have to be considered nondetects in order to make accurate comparisons. Censoring data to a common censoring limit for all pesticides is necessary when making comparisons among pesticides; however, this reduces the amount of detections and restricts the statistical power needed to determine factors affecting an individual pesticide. The pesticide with the highest detection limit is prometon with a limit of 0.018 µg/L. Therefore, a common censoring limit of 0.018 µg/L is used for comparing detection frequencies among pesticides, and the individual censoring limit (table 12) is used for analysis when comparing one pesticide to other variables. The difference in the percentage of detections when using the

Table 11. Selected 1992 pesticide-use estimates for six NAWQA study units with ground-water studies in Piedmont Aquifers.

[lbs, pounds]

Study unit	Pesticide name	Agricultural use rank[1]	Treated area (acres)	Active ingredient applied (lbs)
ACFB[2,3]	alachlor	24	44,531	92,024
	atrazine	8	201,177	310,675
	metolachlor	7	179,486	341,562
	simazine	57	11,852	17,364
DELR[4]	alachlor	5	18,623	34,009
	atrazine	2	164,363	186,703
	metolachlor	1	136,916	239,098
	simazine	12	10,237	13,984
LINJ[1]	alachlor	9	12,200	23,130
	atrazine	6	33,361	47,856
	metolachlor	2	50,510	96,001
	simazine	24	4,117	7,362
LSUS[1]	alachlor	5	95,611	170,215
	atrazine	2	464,013	518,145
	metolachlor	1	425,705	758,897
	simazine	11	82,910	78,509
POTO[1]	alachlor	6	108,853	203,609
	atrazine	4	279,096	377,881
	metolachlor	3	220,810	417,337
	simazine	10	88,938	94,423
SANT[1]	alachlor	8	94,808	144,681
	atrazine	4	172,335	225,912
	metolachlor	12	81,309	114,275
	simazine	24	22,920	37,303

[1]Ranking of agricultural use of pesticide within study-unit boundary in pounds of active ingredient applied.

[2]Data from Michael S. Majewski, U.S. Geological Survey, 1997, written commun.

[3]Study-unit abbreviations are given on table 2.

[4]Data from Gail P. Thelin, U.S. Geological Survey, 2004, written commun.

Table 12. Pesticides and degradates analyzed in ground-water samples from the Piedmont Aquifer System.

[CAS, Chemical Abstract Services Registry; D, degradate, H, herbicide; I, insecticide; µg/L, micrograms per liter; MCL, Maximum Contaminant Level; <, less than; NA, not available]

Pesticide or degradate	CAS number	Type	Class	Maximum concentration (µg/L)	MCL (µg/L)	Individual censoring limit[1] (µg/L)	Number of detections (number of detections using censoring limit of 0.018 µg/L)	Number of samples	Detection frequency using individual censoring limit (percent)
desethyl atrazine	6190-65-4	D	atrazine degradate	1.02	2	0.002	122 (76)	270	45.19
atrazine	1912-24-9	H	triazine	0.72	3	0.001	88 (51)	270	32.59
metolachlor	51218-45-2	H	acetanilide	4.99	NA	.001	36 (21)	270	13.33
simazine	122-34-9	H	triazine	.204	4	.005	26 (12)	270	9.63
prometon	1610-18-0	H	triazine	.315	NA	.018	21(21)	270	7.78
dieldrin	60-57-1	I	organochlorine	.068	NA	.001	17 (9)	270	6.30
alachlor	15972-60-8	H	acetanilide	.249	NA	.002	15 (5)	270	5.56
p,p'-DDE[2]	72-55-9	D, I	p,p'-DDT degradate	.006	NA	.001	8 (0)	255	3.14
carbaryl	63-25-2	I	carbamate	.0908	NA	.003	8 (4)	270	2.96
carbofuran[2]	1563-66-2	I	carbamate	.166	40	.002	5 (2)	255	1.96
diazinon	333-41-5	I	organophosphorus	.0391	NA	.002	4 (1)	270	1.48
tebuthiuron	34014-18-1	H	urea	.41	NA	.010	4 (4)	270	1.48
cyanazine[2]	21725-46-2	H	triazine	.085	NA	.004	2 (1)	255	.78
EPTC[2]	759-94-4	H	thiocarbamate	.008	NA	.002	2 (0)	255	.78
pebulate[2]	1114-71-2	H	thiocarbamate	.052	NA	.004	2 (1)	255	.78
fonofos	944-22-9	I	organophosphorus	.003	NA	.0027	2 (0)	270	.74
metribuzin	21087-64-9	H	triazine	.0103	NA	.002	2 (0)	270	.74
trifluralin	1582-09-8	H	dinitroaniline	.014	NA	.002	2 (0)	270	.74
acetochlor[3]	34256-82-1	H	chloroacetamide	.0365	NA	.002	1 (1)	178	.56
butylate[2]	2008-41-5	H	thiocarbamate	.002	NA	.002	1 (0)	255	.39
linuron[2]	330-55-2	H	urea	.029	NA	.002	1 (1)	255	.39
napropamide	15299-99-7	H	amide	.07	NA	.003	1 (0)	255	.39
terbacil[2]	5902-51-2	H	uracil	.277	NA	.007	1 (1)	255	.39
triallate[2]	2303-17-5	H	thiocarbamate	.001	NA	.001	1 (0)	255	.39
2,6-diethylaniline	579-66-8	D	alachlor degradate	.003	NA	.003	1 (0)	270	.37
benfluralin	1861-40-1	H	dinitroaniline	.0057	NA	.002	1 (0)	270	.37
DCPA	1861-32-1	H	chlorobenzioc acid	.004	NA	.002	1 (0)	270	.37
pendimethalin	40487-42-1	H	dinitroaniline	.009	NA	.004	1 (0)	270	.37
terbufos	13071-79-9	I	organophosphorus	.012	NA	.012	1 (0)	270	.37
azinphos-methyl	86-50-0	I	organophosphorus	<.001	NA	.001	0 (0)	270	.00
chlorpyrifos	2921-88-2	I	organophosphorus	<.004	NA	.004	0 (0)	270	.00
disulfoton[2]	298-04-4	I	organophosphorus	<.017	NA	.0017	0 (0)	255	.00
ethalfluralin[2]	55283-68-6	H	dinitroaniline	<.004	NA	.004	0 (0)	255	.00
ethoprop[2]	13194-48-4	I	organophosphorus	<.003	NA	.003	0 (0)	255	.00
alpha-HCH[2]	319-84-6	I	organochlorine	<.0046	NA	.0046	0 (0)	255	.00
lindane	58-89-9	I	organochlorine	<.004	NA	.004	0 (0)	255	.00

Table 12. Pesticides and degradates analyzed in ground-water samples from the Piedmont Aquifer System.—Continued

[CAS, Chemical Abstract Services Registry; D, degradate, H, herbicide; I, insecticide; µg/L, micrograms per liter; MCL, Maximum Contaminant Level; <, less than; NA, not available]

Pesticide or degradate	CAS number	Type	Class	Maximum concentration (µg/L)	MCL (µg/L)	Individual censoring limit[1] (µg/L)	Number of detections (number of detections using censoring limit of 0.018 µg/L)	Number of samples	Detection frequency using individual censoring limit (percent)
malathion	121-75-5	I	organophosphorus	<0.005	0.2	0.005	0 (0)	270	0.00
methyl parathion	298-00-0	I	organophosphorus	<.006	NA	.006	0 (0)	270	.00
molinate[2]	2212-67-1	H	thiocarbamate	<.004	NA	.004	0 (0)	255	.00
parathion[2]	56-38-2	I	organophosphorus	<.004	NA	.004	0 (0)	255	.00
cis-permethrin	54774-45-7	I	pyrethoid	<.005	NA	.005	0 (0)	270	.00
phorate	298-02-2	I	organophosphorus	<.002	NA	.002	0 (0)	270	.00
pronamide	23950-58-5	H	amide	<.003	NA	.003	0 (0)	270	.00
propachlor[2]	1918-16-7	H	acetanilide	<.01	NA	.007	0 (0)	255	.00
propanil[2]	709-98-8	H	amide	<.004	NA	.004	0 (0)	255	.00
propargite[2]	2312-35-8	I	sulfite ester	<.013	NA	.013	0 (0)	254	.00
thiobencarb[2]	28249-77-6	H	thiocarbamate	<.002	NA	.002	0 (0)	255	.00

[1]Analytical methods varied during the study period creating multiple reporting limits and method detection limits. All values with a less than (<) remark were considered nondetects; all values reported with no remark were considered detections; and all values with an “E” (estimated) remark were considered detections.

[2]The compounds propachlor, butylate, cyanazine, alpha-HCH, p,p'-DDE, parathion, ethalfluralin, terbacil, linuron, EPTC, pebulate, molinate, ethoprop, carbofuran, disulfoton, triallate, propanil, thiobencarb, and propargite were not analyzed in the podldwgs1 study.

[3]The herbicide acetochlor was not analyzed in 1993 and 1994; therefore, the ground-water studies lsuslusag1, lsussus2, potosus1, and potosus2 (92 samples in all) were not analyzed for acetochlor.

common censoring limit of 0.018 µg/L and using the individual censoring limit for each pesticide is illustrated in figure 20.

The highest concentration of any pesticide detected was a concentration of 4.99 µg/L of metolachlor. Concentrations of detected compounds were low; all but four analyses had concentrations of less than 1 µg/L, and none of the concentrations were above the MCLs. Desethyl atrazine (a degradate of atrazine) was the most frequently detected compound, in more than 45 percent of wells sampled (fig. 20). Atrazine, metolachlor, simazine, prometon, dieldrin, and alachlor were each detected in more than 5 percent of samples. These seven compounds were selected for additional statistical analysis to determine the factors that may contribute to transport of these compounds to the aquifers. These pesticides were selected on the premise that their occurrence makes them the most important pesticides, as well as the greater likelihood of being able to analyze data sets with a greater number of detections. Twenty-two other compounds were detected in samples from fewer than 10 wells each, and 19 compounds were not detected. The frequency of detection of pesticides is lower when using the common censoring limit of 0.018 µg/L; however, the pattern is still similar with only slight changes in the order of frequency of pesticide detection.

Some of the variability seen in pesticide detection frequencies can be explained by the type of study where samples were collected. Atrazine is used mostly in agricultural applications, so detection frequencies of atrazine and desethyl atrazine were highest in the areas where the land use is predominantly agricultural (lsuslusag1 and podldwgs1) and lowest where the land use is predominantly urban and suburban (acfblusur1, acfblusur2, and podllusrc1) (table 13). Conversely, dieldrin, which was primarily used in urban applications (dieldrin use was banned in the United States in 1987), was detected more frequently in some of the urban areas. Because the podldwgs1 study focused on areas that were more recently urbanized, the fact that dieldrin was not detected is not surprising, because the previous land use in much of that study area was either agriculture or forest. Metolachlor, simazine, and alachlor, which are all primarily agricultural pesticides, also were detected most frequently in areas with agriculture as the predominant land use. Prometon, which is not used in agricultural applications, also was detected most frequently in areas with agriculture as the predominant land use, but also was detected in urban areas, likely reflecting its application as a general-use herbicide.

Aquifer characteristics, such as permeability and organic content of aquifer materials, and chemical characteristics of the pesticides affect the potential for detecting pesticides and degradates in ground water. Low-permeability soils or a large distance from the land surface to the water table also may retard pesticide transport, whereas aquifers that have characteristics that allow for rapid movement of water from the land surface, such as carbonate aquifers, may increase the transport of pesticides. Pesticide properties such as solubility, soil-water partitioning coefficient, and half-life also affect the potential of detection in ground water. Properties of the seven pesticides selected for statistical analysis have a range of solubilities; dieldrin has the lowest solubility and desethyl atrazine has the highest solubility (table 14). The organic carbon-water partitioning coefficients indicate dieldrin is the most likely to adhere to soils and desethyl atrazine is the least likely to adhere to soils (table 14). Pesticides such as dieldrin may remain bound to organic material or clay in the soil zone and leach out slowly, whereas desethyl atrazine may be more easily transported through the aquifer. Factors that affect the rate of pesticide deg-

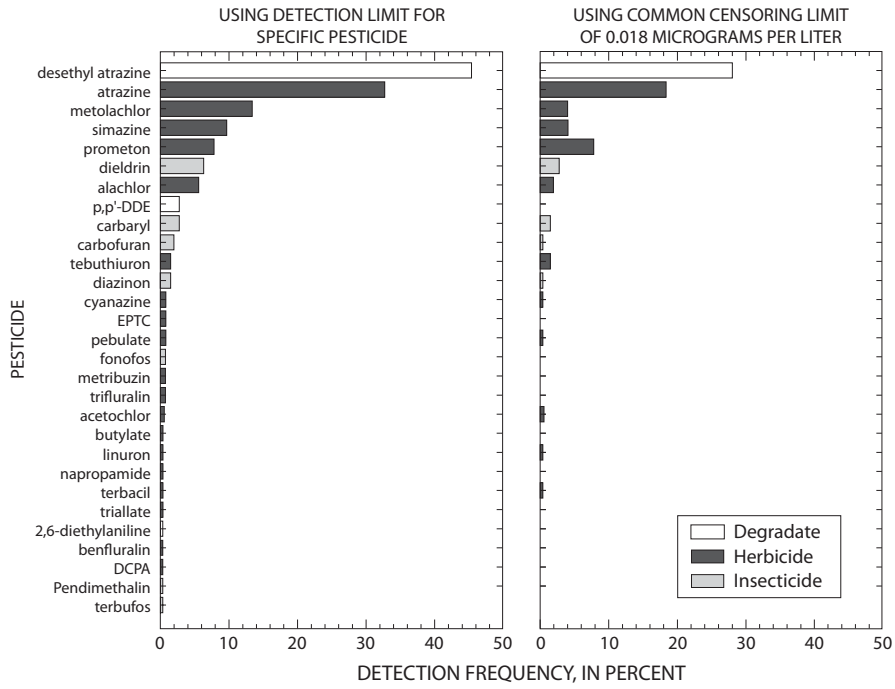

Figure 20. Detection frequency of pesticides and metabolites in ground-water samples from the Piedmont Aquifer System.

Table 13. Pesticide detections from individual well networks in the Piedmont Aquifer System.

Ground-water study-area code[1]	Type of study												
	Urban land use				Agricultural land use	Major aquifer							Drinking water supply
	acfblusur1	acfblusur2	podl lusrc1	Total for urban	lsus lusag1	delr sus1	linj sus3	lsus sus2	potosus1	potosus2	santsus3	Total for major aquifer studies	podl dwgs1
Number of samples	20	17	30	67	30	30	20	30	25	23	30	158	15
Desethyl atrazine	0	0	5	5	24	4	2	20	4	3	2	34	12
Atrazine	0	0	1	1	24	2	0	11	1	1	2	17	9
Metolachlor	0	0	2	2	4	1	0	9	0	1	0	11	4
Prometon	1	0	0	1	8	0	0	0	0	0	0	0	0
Simazine	0	0	0	0	7	1	0	1	0	0	0	2	3
Dieldrin	3	3	0	6	0	1	1	0	0	0	0	2	1
Alachlor	0	0	0	0	2	0	0	2	0	0	0	2	1
Total number of detections[2]	4	3	8	15	69	9	3	43	5	5	4	68	30
Total number of compounds[2]	2	1	3	5	6	5	2	5	2	3	2	6	6

[1]Ground-water study-area codes are defined in table 2.

[2]From the seven compounds listed in the table. Detections are censored to a common censoring limit of 0.018 µg/L.

Table 14. Physical properties of selected pesticides.

[mg/L, milligram per liter; K_{ow}, octanol-water partitioning coefficient, K_{oc}, organic carbon-water partitioning coefficient]

Pesticide name	Physical characteristic		
	Solubility[1] (mg/L)	Log K_{ow}[1]	Log K_{oc}[2]
Dieldrin	0.17	5.4	5.01
Alachlor	240	3.52	3.13
Simazine	550	2.18	1.79
Atrazine	550	2.61	2.22
Prometon	750	2.99	2.60
Metolachlor	1,700	3.13	2.92
Desethyl Atrazine	3,200	1.51	1.12

[1]Solubility and octanol-water partitioning coefficients from National Library of Medicine (2006).

[2]$K_{oc} = 0.041\ K_{ow}$, from Mackay (2001).

radation (microbial, chemical, and photodegradation), as well as rates of adsorption and transfer, also will have an effect on the transport of pesticides to the aquifer (Fishel, 1997). Values for the soil half-life of pesticides, which take into account factors that affect degradation or loss, suggest that the longer it takes a pesticide to degrade, the more likely it is the pesticide will be detected in ground water (Capel and others, 2001); however, using properties such as soil half-life and organic carbon-water partitioning coefficients has been shown to be unreliable to predict pesticide occurrence (Barbash and Resek, 1996). This is probably because of the difficulty in determining a reliable half-life for a pesticide in soils, which may vary more than an order of magnitude depending on environmental factors such as the season (Mackay, 2001).

In general, the pesticides with low solubilities and high organic-carbon partitioning coefficient had a lower percentage of detections (alachlor, dieldrin) and pesticides with higher solubilities and low organic-carbon partitioning coefficients had a higher percentage of detections (desethyl atrazine). It is difficult to draw conclusions about this pattern, however, because of the number of other factors that may affect pesticide occurrence, such as rate and frequency of application, topography, thickness of unsaturated zone, and the relation of land use and aquifer type. The number of pesticides detected in individual wells appears to vary according to the aquifer rock type (figs. 21 and 22); a higher number of pesticides were detected in the carbonate aquifer. However, the carbonate aquifer was the only agricultural land-use study. Carbonate aquifers generally allow for rapid movement of water from the surface and within the bedrock because of solution features, and ground-water flow through crystalline rocks generally is limited to fractures so flow generally is slower in these aquifers. But the study design does not allow a determination of whether land use or aquifer type is the predominant factor in pesticide occurrence.

Factors Affecting Pesticide Detections

Because of the association between land use and pesticide applications (for example, atrazine used on row crops or dieldrin used to treat termites infesting buildings), land use in the recharge area around a well commonly is considered to be a potential factor affecting the presence of pesticides or degradates in ground water. Other potential factors affecting the presence of pesticides or degradates include soil characteristics (such as clay or organic matter content) and aquifer characteristics (such as rock type or depth to the water table).

To determine the relations between pesticide or degradate detections and these various factors, statistical tests were conducted. Kendall's tau correlations were conducted using the ranks of the concentrations of pesticides and individual explanatory variables. Because the number of detections is less than 50 percent for each of the pesticides, the Kendall's tau test is not applicable in the context of a regression but is used in a correlation context (Helsel and Hirsch, 1992). Logistic regression was used to determine associations between occurrence of each of the pesticides and multiple explanatory variables.

Data are ranked for the Kendall's tau test and categorized as detect or nondetect for logistic regression. The individual censoring limit from table 12 is used for censoring each pesticide. For Kendall's tau, values greater than or equal to the respective censoring limits were ranked according to their value, and values less than the respective censoring limit were considered nondetections and assigned a common rank lower than all the detections. Because each pesticide has slightly different detection limits, these statistics represent relations between that pesticide and the selected explanatory variables, and not among the various pesticides. Using a censoring limit common to all pesticides in this analysis would allow comparisons among pesticides but would eliminate valuable data and make the analysis less useful in determining relations between a specific pesticide and the explanatory variables.

Explanatory variables that were considered to have a potential relation to pesticide occurrence were used for the statistical tests. For factors such as land use or soil types, percentages within a 1,640-ft radius of individual wells were used. For other factors, such as well-construction characteristics or water-quality measurements, the actual measured value for the individual wells was used. Initially, the Kendall's tau correlation was conducted on the data set as a whole, but because aquifer type was suspected to be an important variable, additional correlations also were conducted on the data set grouped by aquifer type.

The results of the statistical tests indicate concentrations of atrazine and desethyl atrazine had statistically significant positive correlations to factors associated with agricultural land use (nitrate concentration, percentage of row crop plus hay and pasture, percentage of row crop, percentage of hay and pasture, and estimated amounts of specific pesticides applied) and weak, but negative correlations to urban land-uses (table 15). Kendall's

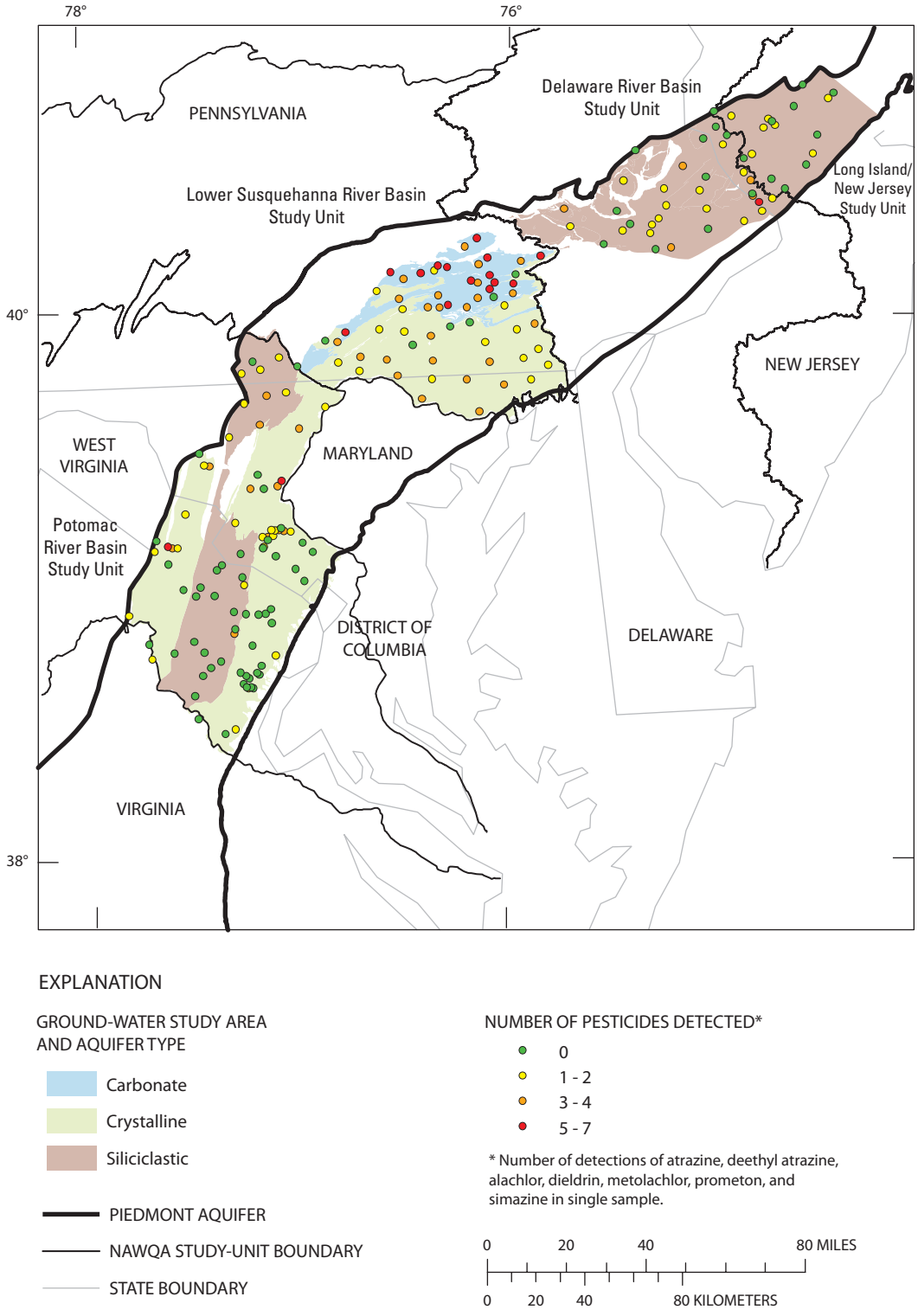

Figure 21. Number of detections of selected pesticides and degradates in ground-water samples from wells in the northern area of the Piedmont Aquifer System, eastern United States.

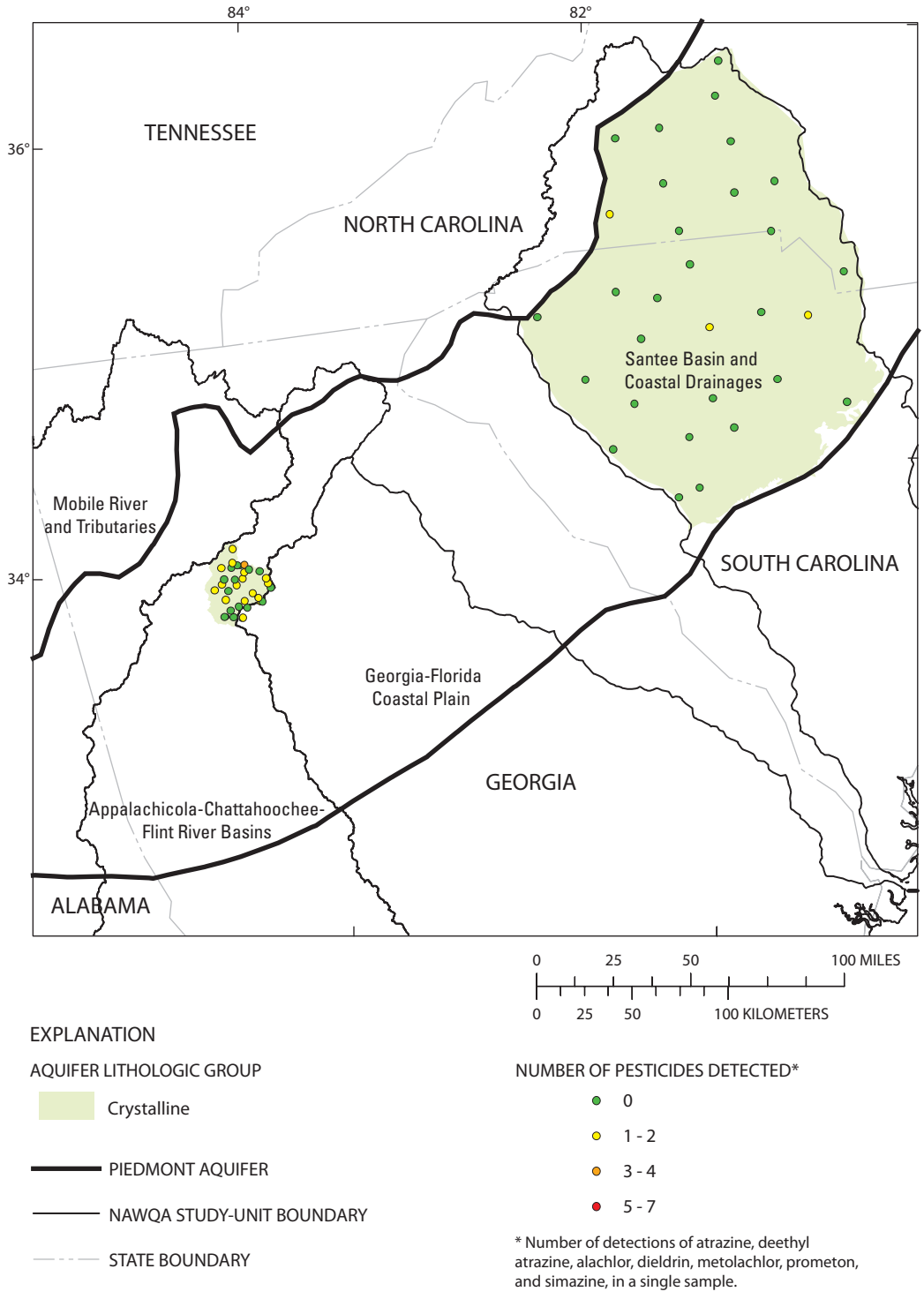

Figure 22. Number of detections of selected pesticides and degradates in ground-water samples from wells in the southern area of the Piedmont Aquifer System, eastern United States.

Table 15. Correlations between atrazine, desethyl atrazine, and atrazine plus desethyl atrazine concentrations in ground water and explanatory variables in the Piedmont Aquifer System by means of Kendall's tau correlation.

[n, number of samples; NS, Correlation not significant at an alpha value of 0.05; X, insufficient data; Carb, Carbonate-rock aquifer; Cryst, Crystalline-rock aquifer; Sil, Siliciclastic-rock aquifer; mg/L, milligrams per liter; kg/yr, kilograms per year; ft, feet; in., inches; in/hr, inches per hour; <, less than]

Factor definition	Median value (all wells)	Kendall's tau coefficients and probability				Kendall's tau coefficients and probability				Kendall's tau coefficients and probability			
		Atrazine				Desethyl atrazine				Atrazine plus desethyl atrazine			
		All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73
Land use[1]													
Low-intensity residential	0.57	-0.22 <.0001	NS	-0.18 .0039	NS	-0.209 <.0001	NS	-0.208 .0005	NS	-0.208 <.0001	NS	-0.198 .0008	NS
High-density residential	.00	-0.14 .0085	NS	NS	NS	-.140 .006	NS	-.143 .028	NS	-.136 .0075	NS	-.137 .035	NS
Commercial industrial transportation	.11	-0.12 .0126	NS	NS	NS	-.140 .0033	NS	-.155 .011	NS	-.135 .004	NS	-.135 .027	NS
Pasture or hay	31.61	.31 <.0001	NS	.394 <.0001	NS	.345 <.0001	-.297 .0213	.406 <.0001	.187 .0322	.345 <.0001	-.299 .0204	.4012 <.0001	.185 .0341
Row crops	2.06	.40 <.0001	.31 .0106	.309 <.0001	NS	.415 <.0001	.316 .014	.368 <.0001	.212 .0182	.414 <.0001	.331 .0102	.352 <.0001	.200 .0250
Urban or recreational grasses	.00	-.22 <.0001	X X	-.224 .0008	NS	-.239 <.0001	X	-.254 <.0001	NS	-.227 <.0001	X	-.230 .0004	NS
Row crop and pasture	40.16	.41 <.0001	NS	.371 <.0001	NS	.430 <.0001	NS	.427 <.0001	.197 .0239	.433 <.0001	NS	.419 <.0001	.192 .0276
Physical and chemical data collected at the time of sampling													
pH	6.3	NS	-.29 .0332	NS	-.215 .0232	NS	-.354 .0097	NS	NS	NS	-.323 .0180	NS	NS
Dissolved oxygen (mg/L)	5.7	.18 <.0001	NS	NS	NS	.266 <.0001	NS	.279 <.0001	.241 .0061	.245 <.0001	NS	.262 <.0001	.230 .0086
Nitrate concentration (mg/L)	1.79	.45 <.0001	.45 .0006	.389 <.0001	.242 .0088	.529 <.0001	.525 <.0001	.397 <.0001	.397 <.0001	.528 <.0001	.544 <.0001	.487 <.0001	.385 <.0001
Chemical use[2]													
Agricultural use of atrazine (kg/yr)	1.095	.33 <.0113	.446 .0136	.348 <.0001	NS	.482 <.0001	.332 .0101	.473 <.0001	.183 .0402	.474 <.0001	.347 .0070	.442 <.0001	NS
Hydrogeology and Soils[3]													
Well depth below land surface (ft)	150	NS	NS	0.143 .0230	NS	NS	NS	.142 .0211	NS	NS	NS	.141 .0206	NS
Casing length	44	NS	NS	NS	-.250 .0234	.132 .0097	.362 .0071	.138 .041	NS	.123 .0156	.305 .022	.144 .0330	NS
Water level in well	26	NS	NS	NS	NS	.125 .0101	.337 .008	.139 .035	NS	.118 .0141	NS	.145 .0278	NS
Hydrologic group A	.00	.22 <.0001	NS	.371 <.0001	NS	.291 <.0001	NS	.440 <.0001	NS	.273 <.0001	NS	.427 <.0001	NS

Table 15. Correlations between atrazine, desethyl atrazine, and atrazine plus desethyl atrazine concentrations in ground water and explanatory variables in the Piedmont Aquifer System by means of Kendall's tau correlation.—Continued

[n, number of samples; NS, Correlation not significant at an alpha value of 0.05; X, insufficient data; Carb, Carbonate-rock aquifer; Cryst, Crystalline-rock aquifer; Sil, Siliciclastic-rock aquifer; mg/L, milligrams per liter; kg/yr, kilograms per year; ft, feet; in., inches; in/hr, inches per hour; <, less than]

Factor definition	Median value (all wells)	Kendall's tau coefficients and probability				Kendall's tau coefficients and probability				Kendall's tau coefficients and probability			
		Atrazine				Desethyl atrazine				Atrazine plus desethyl atrazine			
		All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73
Hydrologic group B	77.08	NS	NS	-0.240 <.0001	NS	NS	NS	-0.249 <.0001	0.228 .0109	NS	NS	-0.240 <.0001	0.244 .0061
Soil thickness (in)	55.42	.04 <.0001	X	.21 .0013	NS	.341 <.0001	X	.274 <.0001	NS	.343 <.0001	X	.249 .0001	NS
Permeability (in/hr)	1.89	-.19 .0001	X	.16 .0182	NS	-.125 .009	X	.161 .153	NS	-.133 .0051	X	.167 .0116	NS
Organic matter	.51	NS	NS	.220 .0003	NS	.090 .044	NS	.270 <.0001	NS	.094 .0368	NS	.265 <.0001	NS
Clay content	22.85	NS	NS	-.277 <.0001	NS	-.170 .0002	NS	-.357 <.0001	-.263 .0033	-.153 .0006	NS	-.345 <.0001	-.275 .0021
Silt content	49.06	.21 <.0001	.28 .0493	.253 <.0001	NS	.254 <.0001	NS	.341 <.0001	NS	.251 <.0001	NS	.322 <.0001	NS
Sand content	30.18	-.11 .0203	-.29 .0493	NS	NS	-.104 .021	NS	NS	NS	-.104 .0195	NS	NS	NS

[1]Data in percent for 1,640-ft radius around well from Vogelmann and others (1998a, 1998b).

[2]Data for 1,640-ft radius around well from Nakagaki (2005).

[3]Average percent soil composition for 1,640-ft radius around well from U.S. Department of Agriculture (2003).

tau correlations also were conducted on the sum of the molar concentrations of atrazine and desethyl atrazine, but the results were fairly similar to those results conducted on the individual compound concentrations (table 15).

Once the data set was separated by rock type, additional correlations were noted. For atrazine and desethyl atrazine, a statistically significant negative correlation for pH was indicated for the subset of samples in carbonate rocks, suggesting atrazine may degrade more quickly in alkaline waters (Fishel, 1997). For desethyl atrazine, fewer correlations were indicated for ground-water samples from carbonate aquifers than for ground-water samples from crystalline aquifers. Correlations between desethyl atrazine and the percentage of pasture were negative for samples from carbonate-rock aquifers but positive for crystalline-rock aquifers. Because atrazine is applied to row crops (mainly corn and soybeans), a negative correlation between the degradate and the percentage of pasture around the well (also seen with atrazine and carbonate) is not surprising. The positive correlation between the degradate and percentage of pasture in crystalline-rock aquifers may be because of the correlation between the land-use categories of row crop and hay and pasture as has been noted previously.

Adding the molar concentrations of atrazine and desethyl atrazine together prior to ranking and rerunning the Kendall's tau test had little effect on the results (table 15). Because most of the wells that contained one of these compounds contained both, combining their molar concentrations may not have changed the outcome of the ranking and, therefore, the outcome of the correlation test. Other studies have indicated the importance of measuring degradate concentrations in ground water (Kolpin and others, 1998), but none of the degradation products of the other frequently detected pesticides were analyzed in a sufficient number of the studies included in this report and so could not be included in any statistical testing.

Correlations for metolachlor were noted mainly in crystalline-rock aquifers (table 16), but the estimated use of metolachlor is greater in three of the study units that have crystalline-rock aquifers (ACFB, LSUS, and PODL) than in the other study units. Again, most of the strongest positive correlations were with agricultural land-use factors and most of the strongest negative correlations were with urban land-use factors. Very few correlations were indicated in siliciclastic-rock aquifers.

Correlations for simazine were noted in carbonate-rock aquifers (table 16). The strongest positive correlations were

Table 16. Correlations between metolachlor, simazine, and alachlor concentrations in ground water and explanatory variables in the Piedmont Aquifer System by means of Kendall's tau correlation.

[n, number of samples; NS, Correlation not significant at an alpha value of 0.05; X, insufficient data; Carb, Carbonate-rock aquifer; Cryst, Crystalline-rock aquifer; Sil, Siliciclastic-rock aquifer; mg/L, milligrams per liter; kg/yr, kilograms per year; ft, feet; in., inches; in/hr, inches per hour; <, less than]

Factor definition	Median value (all wells)	Kendall's tau coefficients and probability				Kendall's tau coefficients and probability				Kendall's tau coefficients and probability			
		Metolachlor				Simazine				Alachlor			
		All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73
Land use[1]													
Low-intensity residential	0.57	-0.147 .0029	NS	-0.148 .0176	NS	-0.129 .0109	NS	NS	NS	-0.104 .0422	NS	NS	X
High-density residential	.00	-.153 .0047	NS	-.199 <.0001	NS	NS	NS	NS	.225 .0424	NS	NS	NS	X
Commercial industrial transportation	.11	-.112 .0261	NS	-.130 .043	NS	NS	NS	NS	NS	NS	NS	NS	X
Pasture or hay	31.61	.243 <.0001	-.276 .0405	.324 <.0001	NS	.186 .0001	NS	.153 .0165	NS	.117 .0186	NS	.159 .0134	X
Row crops	2.06	.339 <.0001	NS	.287 <.0001	NS	.236 <.0001	NS	.150 .021	NS	.246 <.0001	NS	.188 .0041	X
Urban or recreational grasses	.00	-.221 <.0001	X	-.213 .0019	NS	NS	X	NS	NS	-.124 .0286	X	NS	X
Row crop and pasture	40.16	.329 <.0001	NS	.342 <.0001	NS	.248 <.0001	NS	.161 .0112	NS	.205 <.0001	NS	.174 .0064	X
Physical and chemical data collected at the time of sampling													
Dissolved oxygen (mg/L)	5.7	.224 <.0001	NS	.253 <.0001	NS	NS	NS	NS	NS	NS	NS	NS	X
Nitrate concentration (mg/L)	1.79	.371 <.0001	.463 .0007	.329 <.0001	.193 .0437	.271 <.0001	NS	.171 .0102	NS	.248 <.0001	NS	.172 .0100	X
Chemical use [2]													
Agricultural use of pesticide (kg/yr)	1.095	.395 <.0001	NS	.384 <.0001	NS	.261 <.0001	NS	.231 .0005	NS	.257 <.0001	NS	.234 .0004	X
Hydrogeology and Soils [3]													
Well depth below land surface (ft)	150	NS	NS	NS	NS	NS	NS	.139 .0372	NS	NS	NS	NS	X
Casing length	44	NS	NS	NS	-.251 .0276	NS	NS	NS	-.347 .0023	NS	NS	NS	X
Water level in well	26	.102 .0472	NS	.137 .048	NS	.126 .0169	NS	NS	NS	NS	NS	NS	X
Hydrologic group A	.00	.228 <.0001	NS	.424 <.0001	NS	NS	NS	.238 .0007	NS	NS	NS	.187 .0084	X
Hydrologic group B	77.08	NS	NS	-.223 .0003	NS	NS	-.337 .0318	NS	NS	NS	NS	NS	X
Soil thickness (in)	55.42	.347 <.0001	X	.199 .0033	.236 .0307	.221 <.0001	X	NS	NS	.229 <.0001	X	NS	X

Table 16. Correlations between metolachlor, simazine, and alachlor concentrations in ground water and explanatory variables in the Piedmont Aquifer System by means of Kendall's tau correlation.—Continued

[n, number of samples; NS, Correlation not significant at an alpha value of 0.05; X, insufficient data; Carb, Carbonate-rock aquifer; Cryst, Crystalline-rock aquifer; Sil, Siliciclastic-rock aquifer; mg/L, milligrams per liter; kg/yr, kilograms per year; ft, feet; in., inches; in/hr, inches per hour; <, less than]

Factor definition	Median value (all wells)	Kendall's tau coefficients and probability				Kendall's tau coefficients and probability				Kendall's tau coefficients and probability			
		Metolachlor				Simazine				Alachlor			
		All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73
Organic matter	0.51	NS	NS	0.243 <.0001	NS	0.109 .0266	0.49 .0015	NS	NS	NS	NS	NS	X
Clay content	22.85	-.119 .0125	NS	-.351 <.0001	NS	NS	.390 .012	-.144 .0240	NS	NS	NS	-.161 .012	X
Silt content	49.06	.213 <.0001	NS	.303 <.0001	NS	.204 <.0001	.445 .0046	NS	NS	.132 .0079	NS	.133 .0385	X
Sand content	30.18	-.107 .0239	NS	NS	NS	-.161 .0010	-.445 .0046	NS	NS	-.098 .049	NS	NS	X

[1]Data in percent for 1,640-ft radius around well from Vogelmann and others (1998a, 1998b).

[2]Data for 1,640-ft radius around well from Nakagaki (2005).

[3]Average percent soil composition for 1,640-ft radius around well from U.S. Department of Agriculture (2003).

with the average percentage of silt, clay, and organic matter. Clay soils may impede transport of chemicals to the subsurface; therefore, the positive correlation between simazine and clay in carbonate-rock aquifers seems counterintuitive (table 16). Macropore fracturing of clays has been shown to be an important factor in transport of water and contaminants in clay soils in the Piedmont (Radcliffe and West, 2000), thereby potentially increasing the permeability of an otherwise low-permeability setting. The strongest negative correlations were with soil factors associated with high rates of water movement (such as average percentage of sand). Similar correlations for these soils factors were indicated with atrazine in carbonate-rock aquifers. Atrazine and simazine are chemically similar compounds with similar uses, so finding similar correlations is not unusual.

Significant correlations for alachlor were noted mainly in crystalline-rock aquifers (table 16). The strongest positive correlations were with agricultural land-use factors, although weaker than correlations for the other agricultural pesticides. For the entire data set, the strongest negative correlations were with urban land-use factors. Correlations for alachlor in siliciclastic-rock aquifers could not be tested, owing to the lack of detections in those aquifers.

Dieldrin and prometon are pesticides with mainly non-agricultural uses, and the results of the statistical tests reflect this (table 17). Prometon is an herbicide used for highway and utility right-of-ways and around structures. It is not labeled for use on crop land. Prometon is positively correlated to urban land-use factors within crystalline-rock and siliciclastic-rock aquifers but also is positively correlated to agricultural land-use factors when rock type is not considered (table 17). This is likely to be a reflection of prometon's use in both urban and rural settings as a general-use herbicide. Because of concerns over the persistence of dieldrin in the environment, the USEPA banned the use of dieldrin in 1987, and between 1974 and 1987, dieldrin use in the United States was limited to applications for termites in structures. Consequently, the strongest positive correlations were noted with urban land-use factors in crystalline-rock aquifers (table 17). The majority of detections of dieldrin were from ground-water samples from the two urban land-use studies conducted near Atlanta, Ga., where use of dieldrin seems likely. Dieldrin also was the only pesticide to have a significant negative correlation with percentage of organic matter. This is reasonable because dieldrin has a K_{oc} value that is orders of magnitude greater than the other pesticides (table 14), and is therefore more likely to be affected by soil organic matter content.

Logistic regression was used to determine which factors are the most significant in detections of the selected pesticides. Because the pesticide data are highly censored, linear regression was not attempted. The logistic regression was conducted in a manner similar to that done for nitrate. Pesticides data were grouped by 'detect' and 'nondetect' on the basis of the individual pesticide censoring levels (table 12).

A logistic regression model was developed to test the probability that atrazine exceeds 0.0018 µg/L. Results of regression and diagnostics are given in table 18. The significant variables in this model were the application rate of atrazine and the percentage of row crop and hay and pasture in the 1,640-ft radius

Table 17. Correlations between prometon and alachlor concentrations in ground water and explanatory variables in the Piedmont Aquifer System by means of Kendall's tau correlation.

[n, number of samples; NA, Not applicable; NS, Correlation not significant at an alpha value of 0.05; X, insufficient data; Carb, Carbonate-rock aquifer; Cryst, Crystalline-rock aquifer; Sil, Siliciclastic-rock aquifer; mg/L, milligrams per liter; ft, feet; in., inches; in/hr, inches per hour; <, less than]

Factor definition	Median value (all wells)	Kendall's tau coefficients and probability				Kendall's tau coefficients and probability			
		Prometon				Dieldrin			
		All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73
Land Use[1]									
Low-intensity residential	0.57	NS	NS	NS	NS	0.244 <.0001	NS	0.273 <.0001	0.244 .017
High-density residential	.00	NS	NS	NS	.377 .0007	.405 <.0001	NS	.437 <.0001	.339 .0025
Commercial industrial transportation	.11	NS	NS	.191 .0049	.202 .0478	.239 <.0001	NS	.279 <.0001	NS
Pasture or hay	31.61	.174 .0004	NS	NS	NS	-.278 <.0001	NS	-.313 <.0001	-.217 .024
Row crops	2.06	.286 <.0001	NS	NS	NS	-.200 <.0001	NS	-.241 .0002	NS
Urban or recreational grasses	.00	NS	X	NS	.281 .0116	-.340 <.0001	X	.331 <.0001	.339 .0025
Row crop and pasture	40.16	.267 <.0001	NS	NS	NS	-.253 <.0001	NS	-.306 <.0001	-.217 .0246
Physical and chemical data collected at the time of sampling									
pH	6.3	.205 <.0001	-.291 .038	NS	NS	-.133 .0074	NS	NS	NS
Dissolved oxygen (mg/L)	5.7	NS	NS	NS	NS	NS	NS	NS	NS
Nitrate concentration (mg/L)	1.79	.240 <.0001	NS	NS	NS	NS	NS	NS	NS
Population Density[2]									
Population (1990)	98.6	NS	NS	NS	NS	.212 <.0001	NS	.209 .0008	NS
Population (2000)	135.2	NS	NS	NS	NS	.185 .0002	NS	.177 .0045	NS
Hydrogeology and Soils[3]									
Well depth below land surface (ft)	150	NS	NS	NS	NS	-.161 .0019	NS	-.209 .0020	NS
Casing length	44	NS	NS	NS	-.358 .0016	NS	NS	NS	NS
Water level in well	26	NS	NS	NS	NS	-.129 0.0160	NS	NS	NS
Hydrologic group A	.00	NS	NS	NS	NS	-.149 .0087	NS	-.223 .0015	NS

Table 17. Correlations between prometon and alachlor concentrations in ground water and explanatory variables in the Piedmont Aquifer System by means of Kendall's tau correlation.—Continued

[n, number of samples; NA, Not applicable; NS, Correlation not significant at an alpha value of 0.05; X, insufficient data; Carb, Carbonate-rock aquifer; Cryst, Crystalline-rock aquifer; Sil, Siliciclastic-rock aquifer; mg/L, milligrams per liter; ft, feet; in., inches; in/hr, inches per hour; <, less than]

Factor definition	Median value (all wells)	Kendall's tau coefficients and probability				Kendall's tau coefficients and probability			
		Prometon				Dieldrin			
		All wells n=270	Carb n=30	Cryst n=167	Sil n=73	All wells n=270	Carb n=30	Cryst n=167	Sil n=73
Hydrologic group B	77.08	NS	NS	NS	NS	0.262 <.0001	NS	0.347 <.0001	NS
Hydrologic group C	13.00	NS	NS	NS	NS	-.238 <.0001	NS	-.335 <.0001	NS
Hydrologic group D	2.35	-.177 .0006	NS	NS	NS	-.197 .0001	NS	.-282 <.0001	NS
Soil thickness (in)	55.42	-.294 <.0001	X	NS	NS	-.270 <.0001	X	-.378 <.0001	NS
Organic matter	.51	NS	NS	NS	NS	-.183 .0002	NS	-.266 <.0001	NS
Clay content	22.85	.130 .0081	NS	NS	NS	.021 <.0001	NS	.270 <.0001	NS
Silt content	49.06	.228 <.0001	NS	NS	.204 .0374	-.213 <.0001	NS	-.299 <.0001	NS
Sand content	30.18	-.231 <.0001	NS	NS	NS	.106 .0323	NS	NS	NS

[1]Data in percent for 1,640 ft radius around well from Vogelmann and others (1998a, 1998b).

[2] Data from Hitt (2005a).

[3]Average percent soil composition for 1,640-ft radius around well from U.S. Department of Agriculture (2003).

Table 18. Summary of logistic-regression models for pesticide detection probability.

[agricultural, row crop + hay and pasture; well-drained soils, hydrologic group A + hydrologic group B; urban, low-intensity residential + high-intensity residential + commercial, industrial, and transportation; --, no value; <, less than]

Pesticide	Results for variable				Results for model			
	Statistically significant variables	Parameter Estimate	Probability (p-value)	Standardized Coefficient	Percent concordance	Hosmer-Lemeshow p-value[1]	Generalized r-square[2]	Maximum rescaled r-square[3]
Atrazine	intercept	-2.14	<0.0001	--				
	atrazine application rate[4]	.07	.0001	0.69	82	0.75	0.31	0.42
	agricultural land use[5]	.01	.0014	.36				
Desethyl Atrazine	intercept	-8.05	<.0001	--				
	atrazine application rate	.07	.0002	.73				
	percentage sand[6]	.11	.0008	.47	83	.45	.31	.42
	percentage silt	.08	.0012	.42				
	agricultural land use	.02	.0067	.31				
Metolachlor	intercept	-9.50	<.0001	--				
	percentage silt	.12	<.0001	.66				
	soils in hydrologic group B	.03	.0016	.49	87	.58	.31	.47
	metolachlor application rate	.04	.0003	.47				
	soils in hydrologic group A	.05	.0002	.38				
Simazine	intercept	-1.24	.1859	--				
	agricultural land use	.02	.0029	.42	75	.11	.12	.23
	percentage sand	-.07	.0039	-.31				
Alachlor	intercept	-9.59	.0006	--				
	row crop	.05	.0089	.36	88	.69	.10	.30
	soil thickness	.11	.0369	.49				
Prometon	intercept	-2.73	.0616	--				
	agricultural land use	.03	.0039	.68				
	percentage sand	-.13	<.0001	-.53	86	.11	.22	.42
	low-density residential land use	.05	.0055	.50				
	well-drained soils	.02	.0153	.39				
Dieldrin	intercept	-9.17	<.0001	--				
	percentage clay	.18	.0001	.72	91	.80	.14	.36
	urban land use	.05	<.0001	.52				

[1]Hosmer and Lemeshow (1989).

[2]Cox and Snell (1989).

[3]Nagelkerke (1991).

[4]Pesticide application rate estimate for 1,640-ft radius around well from Nakagaki (2005).

[5]Land use percent in 1,640-ft radius around well from Hitt (2004).

[6]Soils data in percent in 1,640-ft radius around well from U.S. Department of Agriculture (2003).

around the well. As previously discussed, model validation was not possible because of the limited amount of data, and predictive maps were not created. Standardized coefficients are given to illustrate which variable has the largest effect on the model. Analysis of Pearson residuals illustrate where the model is particularly weak. These values are calculated by comparing model probability to the actual outcome. A high Pearson residual results from a situation where the probability of a detection is very low, but the pesticide is detected anyway. A large negative Pearson residual is from cases where the predictive model indicates a high probability that the pesticide would be present, but it was not detected. This analysis showed high Pearson residuals in cases where the pesticide-use data indicated very low atrazine use, but atrazine was detected anyway. This result indicates either atrazine use for nonagricultural purposes or migration of atrazine from outside the 1,640-ft radius. Large negative Pearson residuals were noted where land use was agricultural and atrazine application rates were moderate to small, but atra-

zine was not detected. The algorithm for distributing pesticide use from the county level to the area around the well data assumed that the total pesticide use was evenly distributed to agricultural land in the county. Therefore, these nondetects can be an indicator that pesticide use is not uniform across each county. Individual agricultural practices may lead to cases where atrazine was not the pesticide of choice near these sites. It is also likely that hydrogeologic factors at the scale of an individual well are the cause of the incorrect predictions. The complexity of the aquifers makes it quite possible that a pesticide could be transported from an upgradient location outside of the 1,640-ft radius to a well where the digital data predict a low probability of detecting a pesticide. It is also likely that a well that is predicted to have a high probability of having a pesticide detected could have hydrologic factors that inhibit movement of the pesticide to the well.

A logistic regression model also was developed for testing the probability that desethyl atrazine exceeded the detection limit of 0.002 µg/L (table 18). The model created for desethyl atrazine was statistically significant. The significant variables in the regression were the percentage sand, the percentage silt, the application rate of atrazine, and the percentage row crop and hay and pasture in the 1,640-ft radius around the well. This indicates the probability of desethyl atrazine exceeding 0.002 µg/L is greatest in agricultural areas with a high atrazine use and soils with a high silt or sand content. These variables are not the same as those determined for atrazine, and these differences may indicate desethyl atrazine is more persistent in environments with sandy or silty soils. The highest Pearson residuals were in urban areas where atrazine use was reported as being very low or non-existent, yet desethyl atrazine was still detected. This is either an indicator of nonagricultural use of atrazine or possibly the 1,640-ft radius is not a good approximation of the contributing area. Large negative Pearson residuals were in areas with a high percentage of agricultural land use and nondetections of desethyl atrazine, possibly indicating atrazine was not a pesticide of choice in those areas.

The logistic regression model testing the probability of metolachlor exceeding 0.001 µg/L was statistically significant (table 18). The significant variables in the model were the application rate of metolachlor, the percentage of soils in hydrologic group A, the percentage of soils in hydrologic group B, and the percentage silt. This indicates areas with a high application rate of metolachlor, a high percentage of silt, and well-drained soils are the most likely to have metolachlor detected. The highest Pearson residuals were at sites where the application rate of metolachlor is nonexistent or very low, but metolachlor is detected anyway. Many of these sites are in urban areas, and metolachlor use would not be expected, unless it is being used for nonagricultural purposes. The lowest Pearson residuals are in areas where metolachlor use is high, but it is not detected.

The logistic regression models were developed to test the probability of detecting simazine, alachlor, prometon, and dieldrin (table 18). The low number of detections (less than 10 percent) for these compounds may make these models less useful in determining the factors affecting detections of these pesticides than models for atrazine and metolachlor, and the results of regression diagnostics for these four models show a lower predictive power than the models for atrazine and metolachlor. The model for simazine had two significant variables (table 18) — the percentage of row crop and pasture and hay in the 1,640-ft radius around the well and a negative association with the percentage sand. The highest Pearson residuals were for cases with a low amount of agricultural land that had simazine detected. The lowest Pearson residuals were for areas with a high percentage of agricultural land use. Although usage data indicate these areas typically have a high simazine use, use on a specific parcel of land can not be predicted. The negative association between percentage sand and simazine may be because of the interaction between usage patterns and aquifer type. The areas with the highest use of simazine are in the carbonate aquifer, which typically has a low percentage of sand in the soils.

The model for alachlor had two significant variables (table 18)—the percentage of row crop in the 1,640-ft radius around the well and the soil thickness. High Pearson residuals were for sites with a low percentage of row-crop land use that had alachlor detected. The most negative Pearson residuals were for sites with a thick soil profile and a high amount of row-crop land use but did not have alachlor detected. These sites with large negative residuals were in the lsuslusag1 study where use of alachlor is high; however, it may not have been applied in areas near the wells sampled for this study.

Prometon and dieldrin are pesticides with mainly non-agricultural uses, as indicated by the results of the statistical tests (table 18). Prometon is an herbicide used for highway and utility right-of-ways and around structures. It is not labeled for use on crop land. The majority of detections of dieldrin were from ground-water samples from the two urban land-use studies conducted near Atlanta, Ga. The logistic regression model for prometon had four significant variables (table 18)—two land-use categories - low-density residential, and row crop, hay and pasture - as well as two transport categories - a negative relation to the percentage sand, and a positive relation to the percentage of well-drained soils (hydrologic group A and B). The relation between prometon detections and both residential and agricultural land use is consistent with the application of a general-use herbicide on roadsides and vacant lots in many settings. The negative association between prometon detections and percentage sand probably does not imply that prometon does not enter the aquifer when the overburden has a high sand content, rather, it probably is an indication that prometon use is lower in the areas where soils had a higher sand content; or some other unknown factor. The highest Pearson residuals for the model were for cases where there was a very low percentage of either agricultural land use or residential land use, resulting in a low probability value, but prometon was detected. The statistical model seems to require both land-use types for a predicted high probability, but in reality, a high percentage of either land-use type probably increases the likelihood of detecting prometon. The most negative Pearson residuals were for areas with very high percentages of agricultural or residential land, well-

drained soils, and a low percentage of sand, but no prometon-detected. The usage statistics for prometon are not recorded; therefore, these areas may represent cases where prometon use is low or non-existent.

The logistic regression model for dieldrin had two significant variables (table 18)—percentage of urban land use (low-density residential, high-intensity residential, and commercial/industrial) in the 1,640-ft radius around the well and the percentage clay. The higher probability of detecting dieldrin in urban settings is consistent with what is known about the use of dieldrin; however, the higher probability of detecting dieldrin in areas with a higher clay content is somewhat counterintuitive. The positive relation between percentage clay and the detection of dieldrin may be a result of the fact that 14 of the 18 detections of dieldrin were in the urban areas (acfblusur1 and acfblusur2), which also happened to have the highest percentage of clay. It could also be that, in areas with a high clay content, dieldrin may persists longer. The highest Pearson residuals for the dieldrin model were for cases where there was a detection of dieldrin in an area with a low percentage of urban land use. These cases may have been in areas with a small number of homes, but a residual amount of dieldrin in the soil. Other high Pearson residuals were for cases where there was urban land use but a low percentage of clay. The most negative Pearson residuals for the dieldrin model were for areas with a high percentage of urban land use and a high clay content but had no detection of dieldrin. These areas may never have had dieldrin applied, because there are no records of dieldrin use.

In summary, the logistic regression results indicated similar findings for most pesticides. The factors with the largest effect on determining pesticide presence include source factors - such as the actual application rate or a land-use surrogate - and transport factors - such as percentage sand or silt or permeability. Some of the factors vary among pesticides, and a data set with an adequate number of samples in each type of area would be needed to determine if some of the associations (such as the positive association between dieldrin and percentage clay) are useful for predicting pesticide concentrations or are because of a unique characteristic of the data set (if the only areas where dieldrin use was high happened to be in areas with a high percentage of clay).

Volatile Organic Compounds in Ground Water

Volatile organic compounds (VOCs) are man-made chemicals that enter the environment through daily use in commerce, industry, transportation, and agriculture and the daily activities of individuals. Although the term 'volatile' implies preferential partitioning into air from water, these compounds are water soluble, and if introduced into the environment, will be present in ground water.

VOC Sources

In a general sense, where land use is associated with human activity, VOCs are probably in use, and quite often, being unintentionally and intentionally released to the environment, as in the following examples. Localized releases of VOCs to the environment occur by leakage from above- and below-ground storage tanks and by direct application of pesticides, because VOCs are used in the formulation of pesticides (Barbash and Resek, 1996). VOCs also are released to the environment in industrial and automotive exhausts and by leakage of refrigerants and intentional application of fumigants. VOCs released to the environment as exhaust, gases, and aerosol sprays can drift away from their sources as airborne contaminants to have a broader distribution in the environment, including areas where VOCs are not in direct use. VOCs also are produced as disinfection by-products (trihalomethanes) by chlorination of drinking water and can be released to the environment by leakage of treated drinking water from water-distribution pipes or by the use of treated water in lawn-care irrigation. In rural settings, disposal of household chlorine bleach and other chlorinated products through septic-tank systems can result in trihalomethanes that are released through septic drain lines to the environment.

Distribution of Detections of VOCs

To assess the occurrence of VOCs in PAS, water samples from 206 sites, including 187 wells and 19 springs (groundwater discharge), were collected in 9 NAWQA studies ranging from Georgia to New Jersey and were analyzed for 59 VOCs. As with the pesticides, analytical changes during the study period resulted in multiple reporting limits within and among types of VOCs. To allow the maximum amount of data for interpretation, the individual censoring limits for a given VOC are used except when making comparisons among VOCs. The individual censoring limit was 0.2 µg/L for 52 of the 59 VOCs and 0.26 to 1.0 µg/L for 7 VOCs. After censoring, the results included 137 detections of 29 VOCs, 1 or more VOCs were detected in 35 percent of the 206 samples. In 13 percent of the samples, two or more VOCs were detected. Trichloromethane (chloroform) and methyl-tert butyl ether (MTBE) were the only two individual VOCs to be detected in more than 10 percent of the 206 samples (fig. 23). The detection frequency was less than 3.5 percent for each of the other 27 VOCs. Detections of chloroform were more frequent in urban areas in Georgia, Maryland, and eastern Pennsylvania (fig. 24). MTBE was detected in those same urban areas but was also detected in agricultural land-use areas near where the use of MTBE was heaviest, possibly indicating atmospheric sources (fig. 25). To allow accurate comparisons, only those VOCs with a common censoring limit of 0.2 µg/L are shown in fig. 23. This eliminates four detections of dichloromethane above 0.38 µg/L, four detections of dichlorodifluoromethane (freon-12) above 0.27 µg/L, four detections of napthalene above 0.5 µg/L, and one detection of methyl chloride above 0.5 µg/L.

Trihalomethanes (29.2 percent) and solvents (28.5 percent) were the most frequently detected types of VOCs of the 137 detections (fig. 26). Other types of VOCs detected included a gasoline oxygenate (15.3 percent), gasoline hydrocarbons (15.3 percent), refrigerants (8 percent), VOCs used in organic synthesis (2.2 percent), and fumigants (l.5 percent). Land use associated with detections in six of the seven VOC types was predominantly urban (residential). MTBE detections, the only oxygenate detected (one of two analyzed), are almost evenly associated with residential, agricultural, and forested land uses, probably reflecting two methods of release to the environment by localized leakage from storage tanks and distribution as an airborne contaminant in exhaust.

Factors Affecting VOC Detections

The frequency of VOC detection can be partially explained by sample distribution (depth) relative to land surface. Of the 137 detections in 9 NAWQA studies, 60.6 percent were detected in water samples collected from springs at land surface in 1 study and shallow monitoring wells in 2 studies (fig. 27). The monitor wells had median total depths of 31 and 61 ft in the two studies and, therefore, had sample depths closer to the land surface, relative to the public supply and domestic wells in the other six NAWQA studies. The median well depths were 300 ft for the public supply wells used in one study and range from 140 to 200 ft for the domestic wells in the other five studies. Of the 137 detections, 39.4 percent were in water samples collected from the deeper domestic and public supply wells in six NAWQA studies (fig. 27).

The association of VOCs with sample depth relative to land surface also applied in considering the percentage of wells in each of the nine areas with at least one VOC detection (fig. 27). VOCs were detected in greater than 50 percent of the samples collected from springs and monitor wells and in less than 40 percent of the samples in each of the five domestic-well studies. In the public-supply well study, 47 percent of the wells had at least one detection, which contradicts the statement that VOC frequency is associated with well depth. A public-supply well generally produces larger volumes of water at higher discharge rates, relative to a domestic well, and, therefore, draws its recharge from a larger area. Given that public-supply wells are in areas with higher population densities, if the public-supply well is open to the same aquifer at about the same depth as

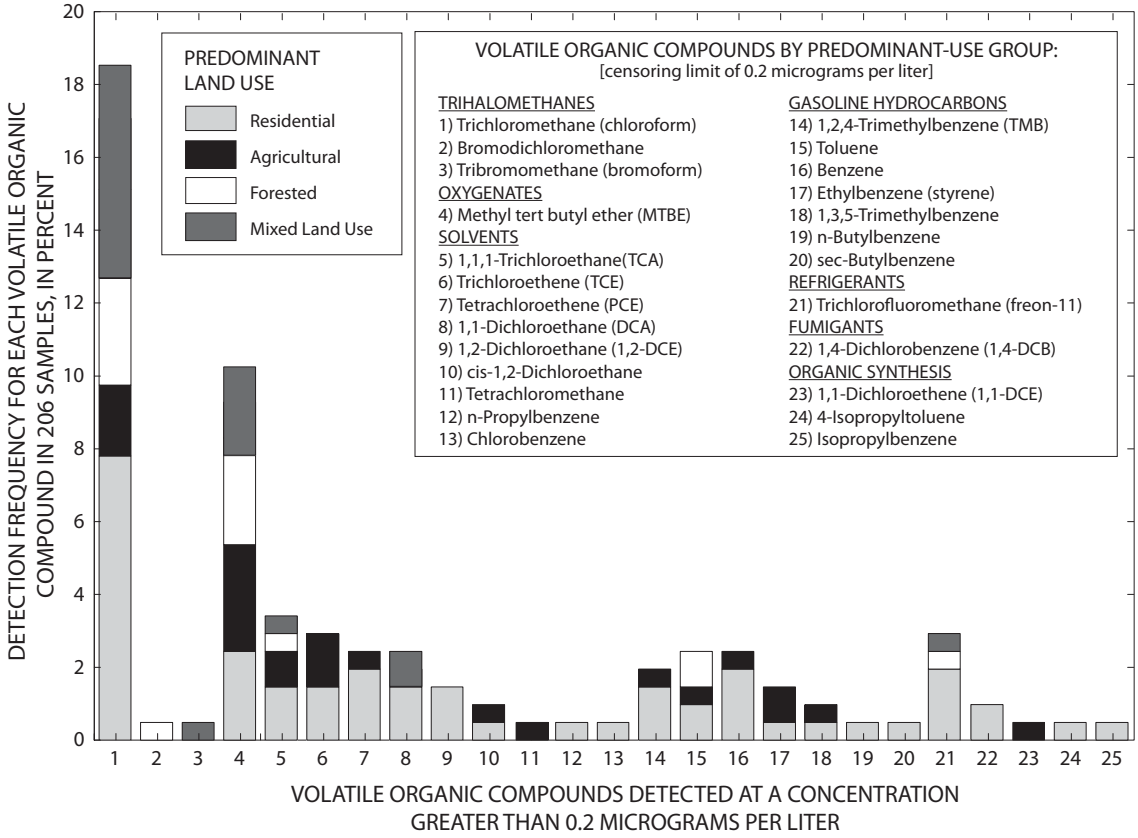

Figure 23. Detection frequency in ground water of the 25 volatile organic compounds with a common censoring limit of 0.2 μg/L for NAWQA studies in the Piedmont Aquifer System, eastern United States.

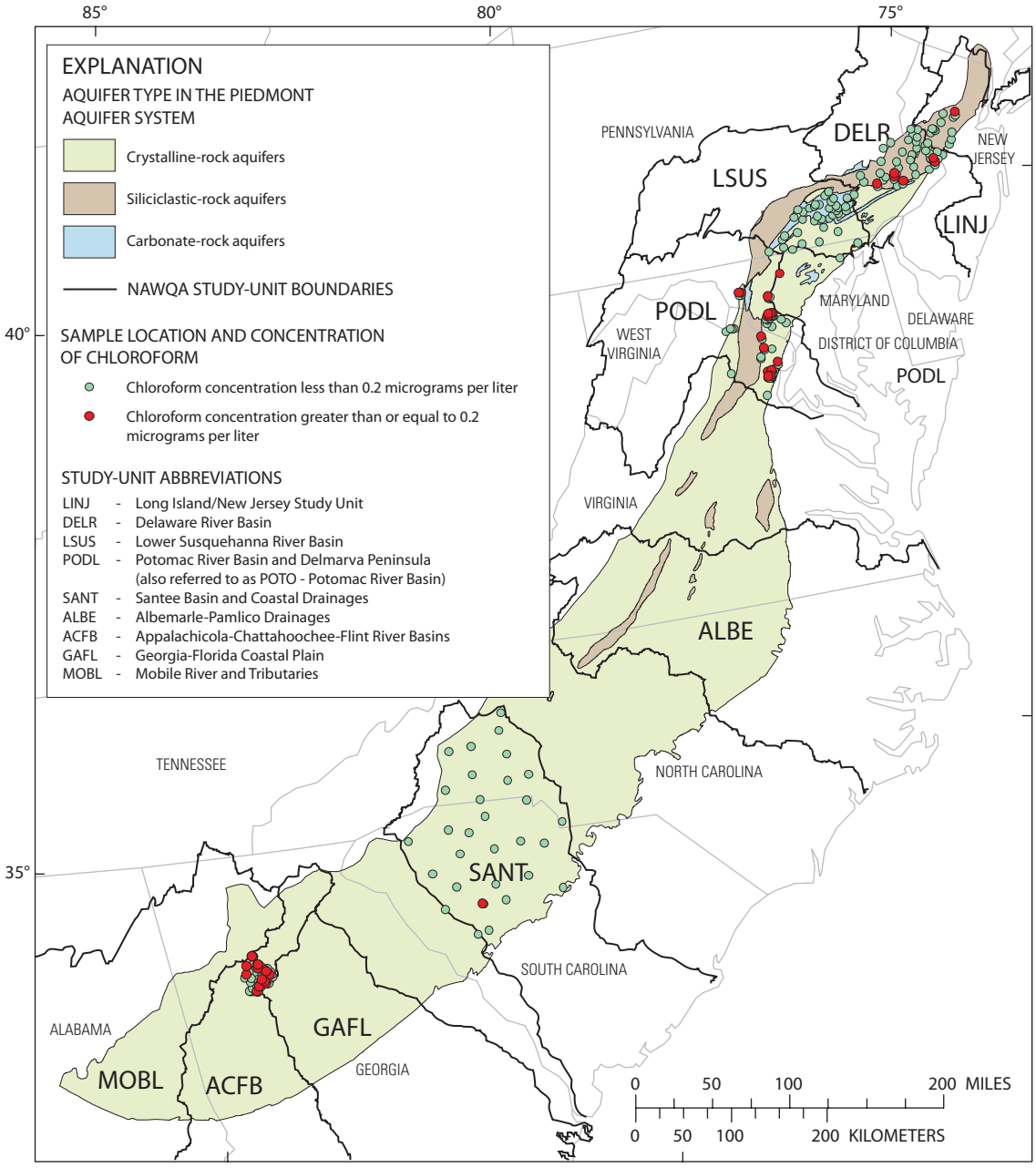

Figure 24. Detections of chloroform in ground water for NAWQA studies in the Piedmont Aquifer System, eastern United States.

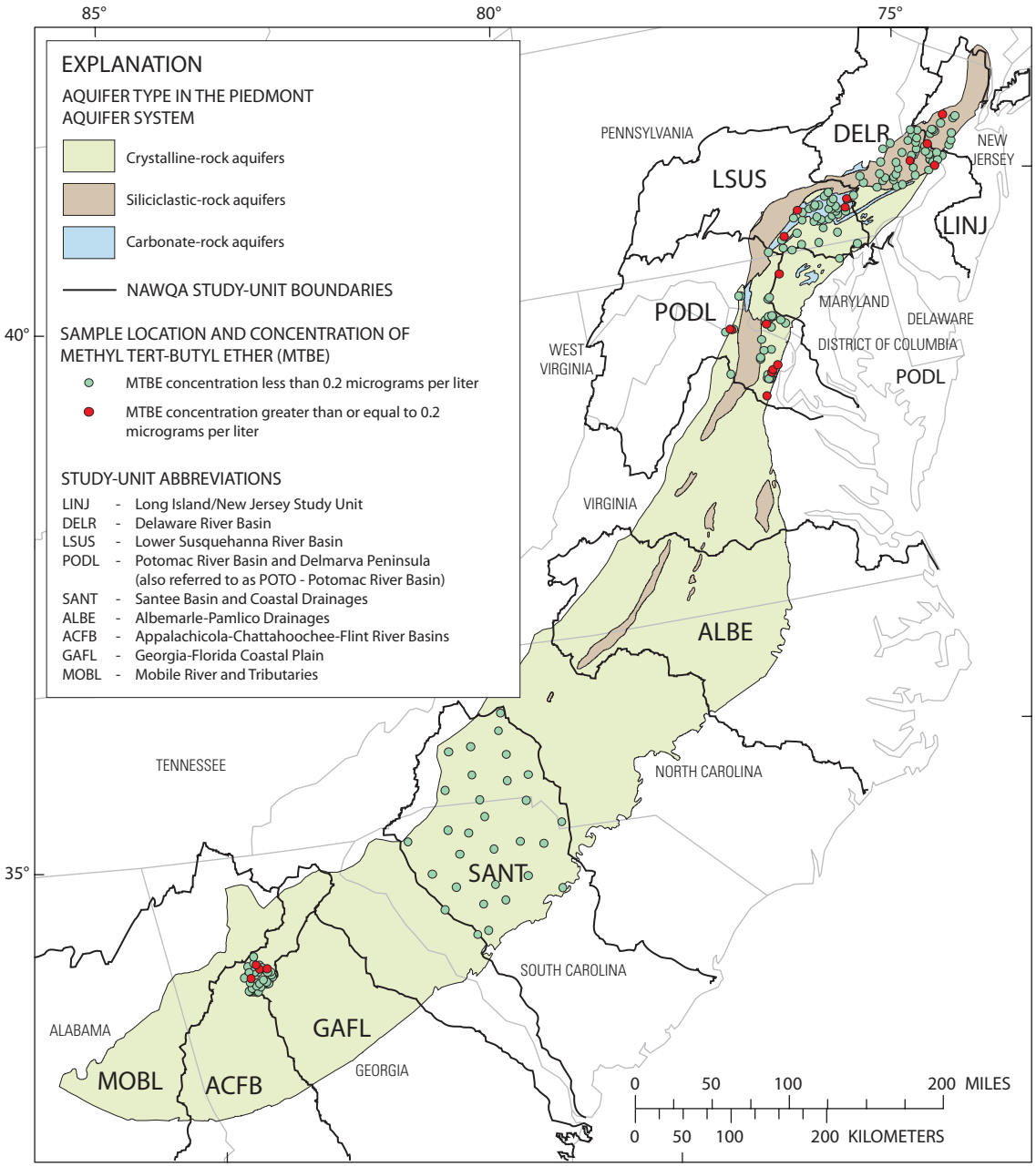

Figure 25. Detections of methyl-tert butyl ether in ground water for NAWQA studies in the Piedmont Aquifer System, eastern United States.

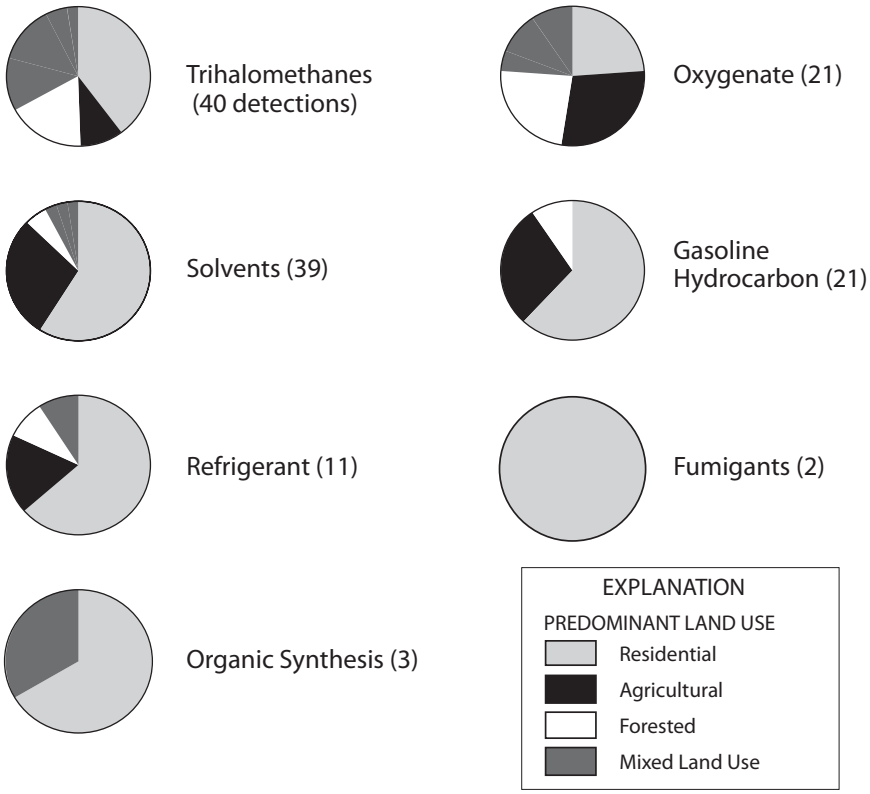

Figure 26. Fraction of all detections associated with predominant land use for seven types of volatile organic compounds, based on results from nine ground-water study areas sampled for NAWQA in the Piedmont Aquifer System, eastern United States.

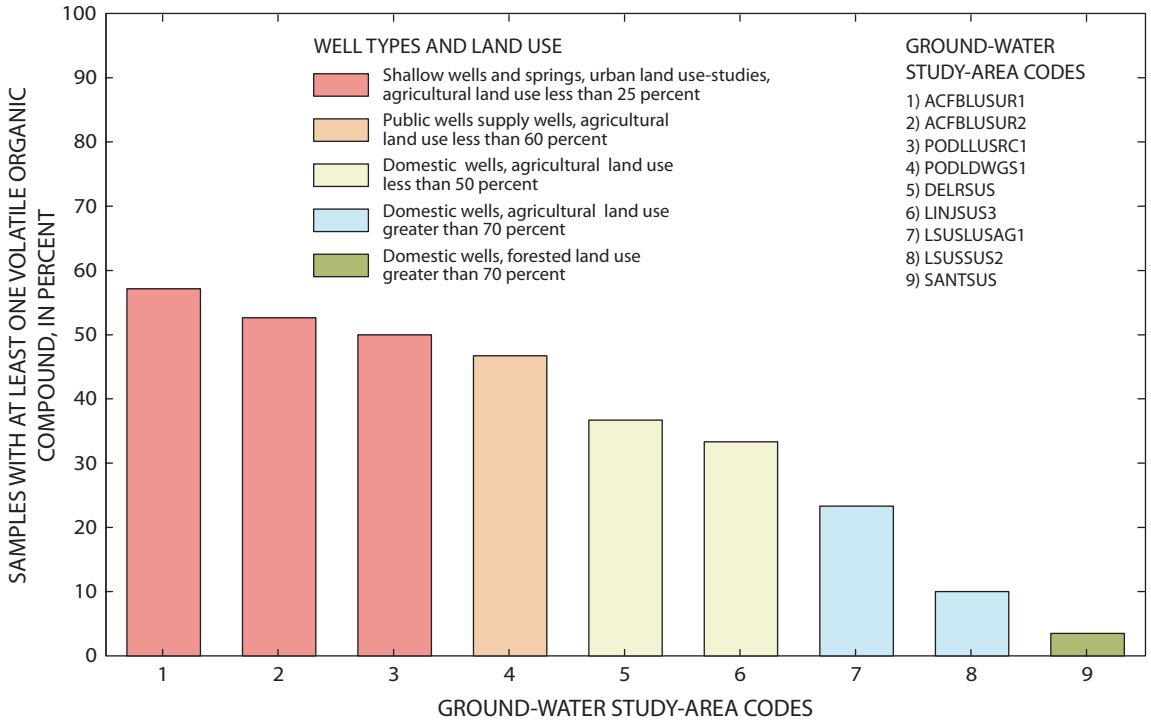

Figure 27. Percent of wells with at least one volatile organic compound detected in each of nine NAWQA ground-water study areas, Piedmont Aquifer System, eastern United States.

the domestic well, and all other environmental conditions are constant, the public supply well is more likely to have detections of anthropogenic contaminants relative to a domestic well.

In addition to sample depth, the frequency of VOC detections for each of the nine NAWQA studies generally can be related to land use. The samples collected in the spring-water study and in one of the shallow monitor-well studies were collected in an urban residential setting with more than 60 percent residential land use and less than 25 percent agricultural land use. These two areas had the highest percentage of samples with at least one detection (fig. 27). Samples collected from shallow monitor wells in this residential study area had slightly more than twice as many of the 137 VOC detections as the samples collected in the other shallow monitor-well study (fig. 27). In eight of the nine NAWQA ground-water study areas, VOC detections generally decreased as the percentage of residential land use decreased and agricultural land use increased (fig. 27). The lowest detection frequency was in the domestic-well study dominated by forested land use. Therefore, VOC use is more commonly associated with residential and agricultural land use and less with forested land use in these PAS study areas but is more common in residential land use relative to agricultural land use.

As with the pesticides, the VOCs were severely censored and were analyzed using Kendall's tau correlations. The logistic regression analysis was performed as previously described, using categories of detect and nondetect of VOCs. The highest common censoring limit for both chloroform and MTBE was 0.2 µg/L, therefore, values greater than or equal to 0.2 µg/L were considered detections and values less than 0.2 µg/L were considered nondetections. In addition to being highly censored, the VOC data set available for analysis was small and limited the likelihood of generating a predictive model. Models tested the likelihood of MTBE and chloroform exceeding 0.2 µg/L. Additionally, a model was created that tested the probability that any one of the VOCs was detected in a well at a concentration of greater than 0.2 µg/L. Because of multiple detections in wells, the variation in detection limits was not a factor in that analysis.

Results of Kendall's tau analysis showed both chloroform and MTBE concentrations had positive correlations with urban land uses such as high-intensity residential and commercial land use (table 19). Chloroform also had a positive correlation with low-intensity residential land use. Both VOCs also had positive correlations with population density and underground storage tanks, and the population on public sewer. The correlation with public sewer and the inverse relation with on-lot septic systems is probably a surrogate for population density. Both chloroform and MTBE had an inverse correlation with well depth, that is, shallow wells had higher concentrations than deeper wells. None of the Kendall's tau correlation coefficients for MTBE exceeded 0.15, which indicates the relation may be statistically significant (based on the p-value) but the predictive value of the relation is weak. Kendall's tau correlation coefficients for chloroform are slightly higher, in the 0.2 - 0.3 range, but still not a strong correlation.

The logistic regression model for chloroform basically supports the generalized assumptions in the previous discussion. The chloroform detections were best predicted by population density (from the 1990 census) and water level (table 20). This model had a concordance of 82 percent and a Hosmer-Lemeshow p-value of 0.38. The generalized r-square value was 0.15, and the maximum-rescaled r-square value was 0.26. The largest Pearson residuals were in cases where the population density was low and chloroform was detected. This is likely to be a result of areas using on-lot sewage-disposal systems. The largest negative Pearson residuals were in areas with a high population density and very shallow water levels. These areas may not have a source of chloroform in the vicinity of the well. The model is useful in identifying those explanatory variables that have the greatest effect on chloroform occurrence, but the regression diagnostics indicate the model is unlikely to be useful for predicting occurrence of chloroform.

The MTBE data set had only 21 detections compared to 38 detections of chloroform. The MTBE model indicated two significant variables, the number of leaking underground storage tanks within a 3,280-ft radius and the percentage of commercial/industrial/transportation land use in the 1,640-ft radius around the well (table 20). The relation between MTBE and commercial/industrial/transportation land use was negative, which is contrary to what would be expected. Upon close examination of the data set, the inverse relation between MTBE and commercial/industrial/transportation land use was driven by a single well where 91 percent of the land use was in the commercial/industrial/transportation category (the highest percentage for any well) but did not have MTBE detected. Without that well in the data set, the commercial/industrial/transportation land-use category is not a significant variable in the regression. Overall, the model was not a good predictor of MTBE detection. The model had only 56 percent concordance, which means that in nearly half of the cases when a detect and a nondetect pair were compared, the nondetect had a calculated probability that was higher than the probability of the detection. The generalized r-square value was 0.06, and the maximum-rescaled r-square value was 0.12. The Hosmer Lemeshow p-value was 0.16. These diagnostics indicate a very weak model that should not be used to predict MTBE occurrence.

Another logistic-regression model was created to test the probability that at least 1 of the 59 VOCs was detected in a well. Seventy-nine wells had at least one VOC detected. The logistic-regression model had two significant variables, the number of leaking underground storage tanks in a 3,280-ft radius, and the population density (from the 1990 census) in a 1,640-ft radius around the well. Given that MTBE and chloroform detections make up about 43 percent of the VOC detections, these results are not surprising. The model had a concordance of 75 percent, and the Hosmer-Lemeshow p-value was 0.23. The generalized r-square value was 0.14, and the maximum-rescaled r-square value was 0.20. The largest Pearson residuals are in locations where the population density is low and with no leaking underground storage tanks in a 3,280-ft radius, with a VOC detected. The explanation of this is probably also because of the presence

Table 19. Correlations between chloroform and methyl-tert butyl ether (MTBE) concentrations in ground water and explanatory variables in the Piedmont Aquifer System by means of the Kendall's tau correlation.

[n, number of samples; NS, Correlation not significant at an alpha value of 0.05; ft, feet; <, less than; UST underground storage tank]

Factor definition	Kendall's tau coefficients and probability	
	Chloroform n=206	Methyl-tert butyl ether n=206
Land Use [1]		
Low-intensity residential	0.197	NS
	.0001	
High-density residential	.303	0.133
	<.0001	.0190
commercial/industrial/transportation	.176	.149
	.0008	.0053
Potential Contaminant Sources		
UST within 3,280 ft of site[2]	.167	.142
	.0023	.0112
Storage tanks within 3,280 ft of site[2]	.145	.132
	.0071	.0163
Density of public sewers [3]	.261	.135
	<.0001	.0073
Density of septic tank or cesspool	-.270	-.133
	<.0001	.0082
Population Density[3]		
Population (1990)	.282	.116
	<.0001	.0215
Population (2000)	.252	.108
	<.0001	.0313
Hydrogeology and Soils		
Well depth (ft below land surface)	-.288	-.210
	<.0001	<.0001

[1]Data in percent for 1,640-ft radius around well from Vogelmann and others (1998a, 1998b).

[2]Data in total number of storage tanks from Price (2005).

[3] Data from Hitt (2005a).

Table 20. Summary of logistic-regression models for chloroform and MTBE detection probability.

[LUST, leaking underground storage tank; --, no value; <, less than]

VOC	Results for variable				Results for model			
	Statistically significant variables	Parameter estimate	Probability (p-value)	Standardized Coefficient	Percent concordance	Hosmer-Lemeshow p-value[1]	Generalized r-square[2]	Maximum rescaled r-square[3]
Chloroform	intercept	-1.20	<0.0199	--				
	water level in well	-.05	.0104	-0.62	82	0.38	0.15	0.26
	population density[4]	.001	.0007	.36				
Methyl-tert butyl ether	intercept	-2.63	<.0001	--				
	LUST in 3,280-ft radius[5]	.42	.0015	.84	56	.16	.06	.12
	commercial/industrial land use [6]	-.15	.0098	.85				
Detection of at least 1 VOC	intercept	-1.37	<.0001	--				
	LUST in 3,280-ft radius[5]	.07	.0020	.41	75	.23	.14	.20
	population density[4]	.0009	.0056	.25				

[1]Hosmer and Lemeshow (1989).

[2]Cox and Snell (1989).

[3]Nagelkerke (1991).

[4]Data from Hitt (2005a).

[5]Data in total number of storage tanks from Price (2005).

[6]Data in percent for 1,640 ft radius around well from Vogelmann and others (1998a, 1998b).

of on-lot sewage disposal systems. The largest negative Pearson residuals were in areas with high population density and numerous leaking underground storage tanks in a 3,280-ft radius. These may be cases where the underground storage tanks were not in the area upgradient from the well. Because of weak regression diagnostics and lack of spatial data on storage tanks, the logistic-regression models for VOCs are not suitable to use for predictive purposes.

Radon in Ground Water

Radon is a colorless, odorless gas that occurs naturally in ground water. It is a radioactive element that decays or breaks down over time to form other elements. Radon has a half-life of 3.8 days (Hem, 1985). The primary health concern related to radon is the inhalation of the decay products of radon. The Surgeon General of the United States has recognized radon as the second leading cause of lung cancer (U.S. Environmental Protection Agency, 1992). Radon gas commonly enters the air in buildings through the basement; however, radon dissolved in ground water can transport additional radon into buildings. Radon is soluble in water yet is easily released back into the air when discharged from faucets or showers. Because radon in indoor air can be from soil gas or ground water, the USEPA proposed rules for radon in ground water include a MCL of 300 pCi/L and an alternative maximum contaminant level (AMCL) of 4,000 pCi/L. The AMCL applies to public water supplies that enact a Multimedia Mitigation plan to address indoor radon; public water supplies that do not enact these measures will be required to meet the MCL of 300 pCi/L (U.S. Environmental Protection Agency, 1999). Radon data were not collected in all the study areas. No radon data exist for the following study areas: linjsus3, podllusurc1, and podldwgs1. Radon data were available for acfblusur2; however, because that was a study of springs, it was not included in the comparison of radon data.

Radon Sources

The source of radon is the radioactive decay of uranium; therefore, rocks with greater uranium content commonly would have higher amounts of radon than rocks with lower uranium content. Rocks such as granites, dark shales, sedimentary rocks with phosphates, and metamorphic rocks derived from those rocks have higher than average uranium content (Otton and others, 1992). With respect to the three aquifer types based on general rock types, uranium content (and thus potential for radon) varies within the general categories. For example, the siliciclastic-rock aquifers include sandstone and shale bedrock, but these two rock types have low and high uranium contents, respectively (table 21). For the most part, siliciclastic-rock aquifers were categorized as shale or mixed sandstone and shale. Crystalline-rock aquifers include granite, ultramafic rock, and basalt, which also have a large range of uranium content. Many of the crystalline rocks are metamorphic, with parent rocks being metasedimentary or metaigneous. Water from wells in metamorphic-rock aquifers that originated from shales and granites would be expected to have higher radon concentrations than water from wells in metamorphic-rock aquifers that originated from basalt or sandstone. The majority of the crystalline rocks in this study are felsic igneous rocks or metamorphic rocks with felsic origin. Those crystalline rocks that are of mafic origin are classified separately for the analysis of radon.

Table 21. Average uranium content in earth's crust, sedimentary, and igneous rocks (modified from Durrance, 1986).

Rock type	Classification in this report	Uranium content (parts per million)
Earth's crust		2.7
Sandstone	Siliciclastic	.45
Shale	Siliciclastic	3.7
Limestone	Carbonate	2.2
Basalt	Crystalline	1.0
Ultramafic rock	Crystalline	.003
Granite	Crystalline	3.0

Distribution of Radon Concentrations

The concentrations of radon in ground water are related to the general bedrock types. In general, water from wells in the crystalline-rock aquifers had higher concentrations of radon than water from wells in the other bedrock aquifers (fig. 28). Because the concentrations of uranium have a relation to lithology that is more specific than the general rock-type groupings (table 21), those groupings have been further subdivided. The crystalline rocks that have more felsic minerals (granite or metamorphic rocks originating as shales—lsussus2, potosus1, and santsus3) had the highest concentrations of radon. The western part of potosus1 is in an area underlain by mafic bedrock and, for purposes of comparing radon concentration, is classified as potosus1w. This area had the lowest median concentration of radon. The samples from acfblusur1 were from very shallow wells with the shallowest water levels (fig. 14). Senior (1998) also noted an association between a lower depth to water and lower radon concentrations in the PAS, possibly explaining the lower concentrations of radon in that area. Samples from delrsus1 and potosus2 had concentrations of radon typically lower than concentrations from samples in the felsic rocks and higher than concentrations in carbonate rock. The siliciclastic rocks were mostly classified as shale or mixed sandstone and shale lithologies. Water from wells in the carbonate-rock aquifer had relatively low concentrations of radon; however, the median concentration was still well above the MCL of 300 pCi/L. The carbonate rocks were primarily limestone lithology, which has a uranium content lower than that of shale or granite. Nearly 80 percent of the samples had radon concentrations between the proposed MCL of 300 pCi/L and the AMCL of 4,000 pCi/L.

Factors Affecting Radon Concentrations

A more detailed analysis focusing on the lithology specific to each sample illustrates the relations between lithology and radon concentration (table 22). The results show the felsic crys-

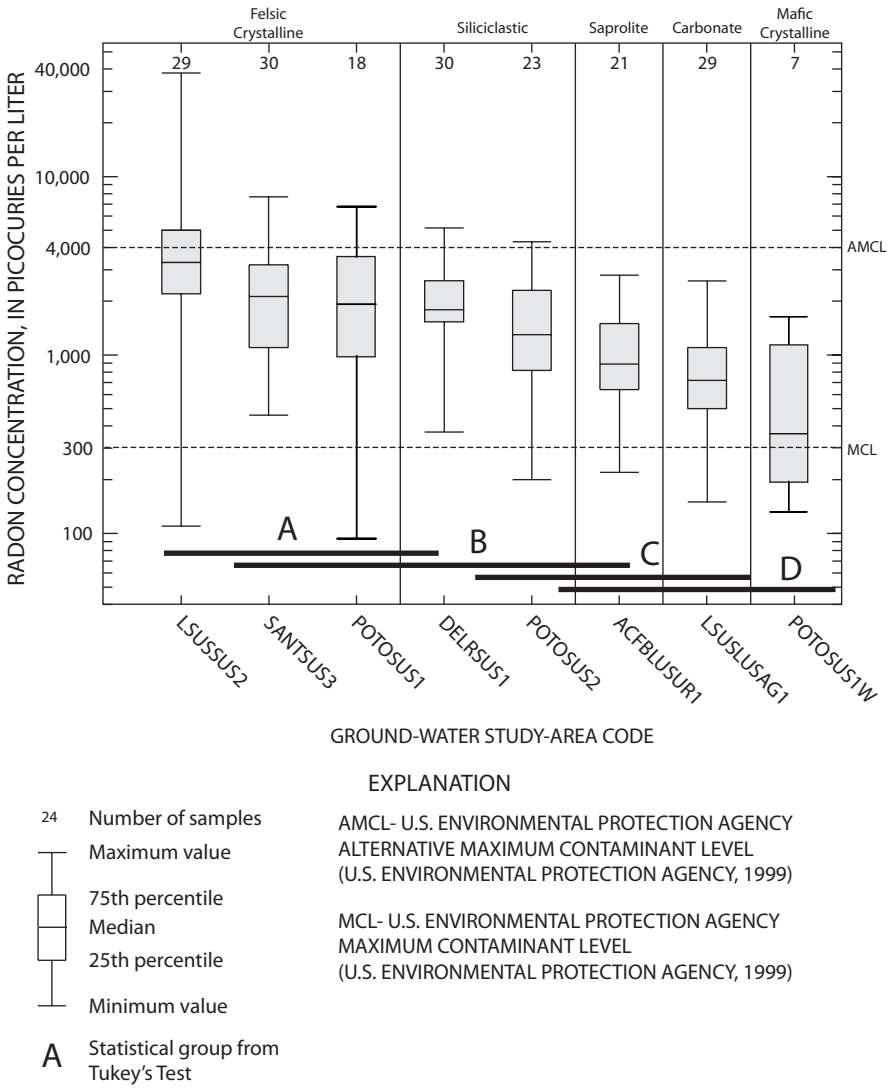

Figure 28. Distribution of concentrations of radon in ground water in subunits of the Piedmont aquifers, and statistical groupings from Tukey's Test (Tukey, 1977). (Ground-water study-area codes are defined in table 2.)

talline rocks have the highest mean radon concentrations, the shales have slightly higher concentrations than the mixed sandstone/shale group, and the carbonates (limestone and dolomite) and mafic metamorphic rocks (greenstone) have the lowest mean radon concentrations. The wells identified as saprolite originated from and overlie felsic-crystalline-rock aquifers. The lower concentrations in saprolite relative to the other felsic-crystalline rocks are unknown but may be related to the shallow nature of these wells and the greater likelihood of exchange of radon with the atmosphere (median difference between water level and total depth of well was only 9.8 ft) or possibly that uranium has been weathered out of the saprolite. Determining the specific cause of the lower concentrations of radon in saprolite is beyond the scope of this project.

Table 22. Median concentrations of radon in water from wells by lithology.

[NA, not applicable]

Mineralogic/ lithologic association	Lithology	Median radon concentration	Number of samples
Felsic crystalline	Schist	3,639	27
Felsic crystalline	Quartzite	2,725	4
Felsic crystalline	Metamorphic (Undifferentiated)	2,370	43
Siliciclastic	Shale	1,928	23
Siliciclastic	Sandstone and Shale	1,886	22
Felsic crystalline saprolite	Saprolite (weathered from schist, gneiss, or granite)	1,228	36
Carbonate	Dolomite	913	6
Carbonate	Limestone	864	23
Mafic crystalline	Greenstone	138	4

Although general patterns in the occurrence of radon can be determined, the variability in radon concentrations also is great. Most of the areas sampled had a broad range of concentrations of radon. In some cases, higher concentrations can be linked to specific geologic formations known to have high uranium content; however, predicting concentrations at a specific location is not feasible. Correlation of radon concentrations to concentrations of other radiochemcial constituents in water is commonly weak, because radon is derived from radium-226, which is in the solid phase in the aquifer materials. A study of radon in ground water in the PAS in Pennsylvania by Senior (1998) in Chester County, Pa., had results similar to the results for the current study. Wells completed in granites and schists typically had higher concentrations of radon than water from wells completed in carbonate or mafic rocks. Senior found a temporal variation of about a factor of two in radon concentrations. The heterogeneity of radon concentrations is such that Senior and Vogel (1995) found variations of up to an order of magnitude in closely spaced wells in a similar hydrogeologic setting. Concentrations of the radiochemical precursors of radon in sedimentary rocks are related to the parent rocks from which the sediments were derived, which may vary locally in concentration. Therefore, although general patterns indicate higher concentrations of radon in felsic crystalline-rock aquifers than in water from other bedrock aquifers, no method exists that would allow prediction of radon concentrations in an individual well.

Limitations of Water-Quality Data and Recommendations for Future Study

Determination of the factors affecting water quality in the PAS is limited by several issues. These include limited spatial coverage, a lack of 'end members' for land use and aquifer-type combinations, and detection limits that change over time. The spatial distribution of sampling is particularly evident in the southern part of the PAS (figs. 6, 13). The areas of the PAS in the MOBL, GAFL, and ALBE study units are completely unsampled, and the ACFB only has samples in an urban area of the PAS. Siliciclastic-rock aquifers are only sampled in the northern study units. Some areas are not covered by NAWQA studies, the largest and most important of which are the area between the POTO and ALBE, and the area between the ALBE and SANT study units. Spatial gaps in NAWQA sampling of the PAS would be covered best by additional sampling in the ALBE and possibly a combined study of the PAS in the MOBL, ACFB and GAFL study units. Because these studies were not designed for regional analysis of the PAS, numerous combinations of land use and bedrock type are not represented by this data set (table 6). Shallow wells in urban areas underlain by crystalline bedrock are well represented, as are domestic supply wells in agricultural areas underlain by carbonate bedrock. Most of the other studies are of mixed land uses, which leads to a small range of land-use types, and a subsequent lack of power to analyze statistical relations between aquifer type, land use, and well depth. Regional understanding of ground water in the PAS would be enhanced by additional studies of urban and agricultural land use in siliciclastic-rock aquifers and agricultural land use in crystalline-rock aquifers. The change in detection limits during the study period also limits the statistical power of the data analysis. For example, MTBE was reported as a detection in 58 wells; however, only 21 of the detections were above the highest common detection limit, which eliminated 37 low-level detections from the data analysis. Some constituent groups were not included in this report because not all the networks had included them in their sampling. For example, trace elements were only analyzed in slightly more than half of the sites. Resampling of earlier study areas for all constituents with the new lower detection limits would increase the statistical power to determine factors affecting water quality in the PAS.

Summary and Conclusions

The National Water-Quality Assessment (NAWQA) Program of the U.S. Geological Survey (USGS) has conducted studies of ground-water quality throughout large parts of the United States. This report is a compilation and analysis of the data for ground-water samples collected by the NAWQA study units in the Piedmont Aquifer System (PAS) of the eastern United States. Samples were collected from 255 wells and 19 springs for numerous analytes within 11 study areas in the PAS. The studies included urban and agricultural land uses, major aquifers, and drinking-water supplies. Samples were collected from the three major aquifers types: crystalline, carbonate, and siliciclastic. Descriptive and statistical analysis of data from 11 studies in the PAS provide the basis for examining the factors affecting ground-water quality. The three major aquifer types in the PAS have different characteristics, many of which are related to lithology, structural geology, and weathering processes.

The study area was subdivided on the basis of lithology. The characteristics of crystalline-, carbonate-, and siliciclastic-rock aquifers were thought to be the most logical basis for analyzing the water-quality data. The crystalline-rock aquifers underlie the largest area in the PAS. On the basis of previous studies, crystalline-rock aquifers were determined to have two major components controlling ground-water flow— the unconsolidated regolith and the fractured bedrock. In some areas, particularly the southern Piedmont, a material called saprolite is also a part of this flow system. This is bedrock that has weathered in place but maintains the original fabric of the rock. In addition, a transition zone between weathered bedrock and fractured bedrock is an important part of the flow system. The carbonate-rock aquifers underlie a small area but are important aquifers in the PAS. The carbonate-rock aquifers are characterized by highly weathered bedrock, and conduit flow can be a factor in the movement of ground water. The presence of solutionally enlarged fractures and conduits can allow rapid transmission of contaminants from the land surface to the aquifer. Dissolution of the minerals in the carbonate bedrock results in ground water with high alkalinity and total dissolved solids, and a stable, near-neutral pH. The siliciclastic-rock aquifers are a relatively small part of the PAS, but locations in the more urbanized parts of the PAS make these aquifers an important resource for water supply. Ground-water flow is controlled by fracture patterns. Because the fracture patterns are related to stress patterns and to the strike of the geologic formations, these aquifers commonly are anisotropic. The siliciclastic-bedrock aquifer includes areas where diabase (a crystalline rock) intrudes into the siliciclastic rock. Because the diabase areas were not sampled, this subdivision is termed the siliciclastic-rock aquifers.

The well networks sampled for this study represented several different combinations of lithology and land use, allowing analysis of the interaction of these factors on water quality. Three studies were conducted in urban areas underlain by crystalline bedrock; two of these urban studies focused on water from the saprolite overlying the fractured bedrock. The study in the carbonate bedrock was also a land-use study that focused on agricultural areas. Of the seven remaining studies, six were in major aquifers with a range of land-use types. Three major-aquifer studies were in crystalline aquifers, and three were in siliciclastic aquifers. The final study was a drinking-water supply study in the crystalline-rock aquifer that focused on deeper wells used for public supply. The well networks did not cover every possible combination of land use, aquifer type, and well depth; therefore, conclusions about these studies are mainly applicable to the specific areas studied. Analysis of water-quality data focused on four constituent groups analyzed in nearly all the studies—nitrate, pesticides, VOCs, and radon.

Nitrate was present in nearly all the samples, but the distribution of concentrations exceeding 10 mg/L was uneven. The USEPA drinking-water standard of 10 mg/L was exceeded in 60 percent of the wells in the lsuslusag1 study and 30 percent of the wells in the lsussus2 study. In all the remaining areas of the PAS, the 10 mg/L standard was only exceeded in 1 percent of the wells. The fact that the lsuslusag1 study is an agricultural land-use study in a carbonate-rock aquifer that is vulnerable to contamination makes this area an anomaly when compared to the rest of the PAS. The vulnerability of aquifers in the lsussus2 study area is not likely to be appreciably greater than any other areas underlain by crystalline-rock aquifers, but this area had a nitrogen input that, although smaller than the nitrogen input for the carbonate-rock aquifer, was nearly double the input of any of the other areas studied. The factors affecting nitrate concentration as determined by the Kendall's tau correlation included numerous source factors; higher agricultural land use and nitrate load were significantly correlated with higher nitrate concentrations. The transport factors affecting nitrate concentration included dissolved oxygen concentration, depth to water, and soil-matrix characteristics. To determine which of these factors had the most effect on nitrate concentration, a linear regression model and two logistic regression models were created. The linear regression model determined three statistically significant variables controlling nitrate concentration: the percentage of agricultural land use, the input of nitrogen from all sources, and dissolved oxygen. The logistic regression models were used to test the probability that nitrate concentration would exceed 4 mg/L. The first logistic regression model started with all variables found to be significant in the Kendall's tau correlation. This model determined that the percentage of agricultural land use, the input of nitrogen from all sources, and dissolved oxygen were the most significant factors in determining nitrate concentration. The second model used only variables that could be mapped spatially, and this model indicated that a higher percentage silt, higher total nitrogen load from all sources, higher percentage agricultural land use, higher percentage sand, and lower percentage organic matter were the factors that had the most influence on nitrate concentration. Although predictive maps were not made, these factors can be used to determine those areas where higher nitrate concentrations are likely to occur.

Data from the PAS for pesticide analysis included samples from 253 wells and 19 springs for 47 pesticides and degradates. The most frequently detected pesticides were atrazine, metolachlor, simazine, alachlor, prometon, dieldrin, and the atrazine degradate, desethyl atrazine,. Data analysis focused on these seven pesticides and degradates. Some of these frequently detected pesticides are widely used in the PAS; others, such as dieldrin, are no longer in use but are persistent in the environment. Pesticide detections followed a general pattern of application and aquifer susceptibility. The largest number of detections of agricultural herbicides was in lsuslusag1, which is the aquifer type most susceptible to contamination and has the highest percentage of agricultural land. The largest numbers of detections of the insecticide dieldrin, which, when in use, was applied to foundations of structures, were in the two urban areas, acfblusur1 and acfblusur2. Kendall's tau correlation tests comparing concentrations of the most frequently detected pesticides to various source and transport factors resulted in numerous significant correlations. Source factors such as the percentage of agricultural land around a well (for agricultural pesticides), application rate of pesticides, and population density (for urban-use pesticides) typically were correlated to higher pesticide concentrations. Transport factors such as aquifer susceptibility to contamination, depth to water, and percentage of well-drained soils, sand, or silt typically were correlated with higher pesticide concentrations. Logistic regression models were created for each of the six most frequently detected pesticides. The logistic regression model for atrazine indicated the percentage of agricultural land use and the application rate of atrazine were the most significant variables in determining whether atrazine would be detected. The logistic regression model for desethyl atrazine indicated those same variables, plus percentage sand and percentage silt, were the most significant factors in determining whether desethyl atrazine would be detected. The model for metolachlor had four variables that were significant in determining detections of metolachlor—application rate, percentage of soils in hydrologic group A, percentage of soils in hydrologic group B, and percentage silt. The model for simazine had two significant variables— the percentage of agricultural land use and the percentage sand in soils. The two significant variables in the logistic regression model for alachlor were soil thickness and the percentage of row-crop land use near the well. The logistic regression model for prometon had four significant explanatory variables— a positive relation between detection of prometon and low-density residential land use near the well, row crop hay and pasture near the well, and the percentage of well-drained soils near the well, and a negative relation between detection of prometon the percentage sand in soils near the well. The model for dieldrin indicated the total amount of urban land and the percentage clay were the most significant factors affecting the detections of dieldrin. The relation between the detection of dieldrin and the percentage clay may be because of the persistence of dieldrin in clay but could also be related to macropore fracturing of clay soils or the typically higher clay content in the urban areas sampled than the more rural areas sampled.

VOCs samples were collected at 206 sites in the PAS and analyzed for 59 compounds. A total of 137 VOCs were detected, and at least one VOC was detected in 79 of the wells. Because of analytical changes during the study period, a range of detection limits was used. To make comparisons valid among these studies, detections were censored to a common limit of 0.2 µg/L. The most commonly detected types of VOCs were classified as trihalomethanes and solvents. The two most frequently detected VOCs were chloroform, a trihalomethane, and MTBE, a fuel oxygenate. In general, detections of VOCs were related to residential land use and shallow well depth. Kendall's tau correlations comparing VOC concentration to various explanatory factors indicated an association between chloroform concentration and urban land uses, leaking underground storage tanks, population density, well depth, and water level. The probability of detecting at least one VOC in a well was greater in areas with high population density and a high number of underground storage tanks. Correlations between MTBE concentration and explanatory variables indicated significant relations between MTBE and urban land use, population density, well depth, and leaking underground storage tanks within a 3,680-ft radius. Logistic regression models were developed for MTBE and chloroform determining the probability that the VOC would be detected at a concentration of greater than 0.2 µg/L. The model for MTBE indicated the probability of detecting MTBE was most significantly related to a higher number of leaking underground storage tanks and a smaller percentage of commercial/industrial/transportation land use near the well. This model, however, was considered very weak statistically. The model for determining the presence of chloroform indicated the probability of detecting chloroform was related to population density and the water level in the well.

Radon was also sampled in a large number of wells. The concentration of radon was found to be related to lithology. The stratification of the PAS into crystalline-rock, carbonate-rock, and siliciclastic-rock aquifers was not adequate for analysis of radon. The parts of the crystalline-rock aquifers underlain by mafic crystalline rocks were analyzed separately for this study. In general, wells in areas where the bedrock was felsic had higher radon concentrations. Siliciclastic-rock aquifers were not further subdivided because nearly all the wells were completed in areas with shale. Radon concentrations in the siliciclastic-rock aquifers were slightly lower than concentrations of radon in water from the felsic crystalline rocks. Carbonate-rock aquifers tended to have radon concentrations slightly lower than concentrations in the shale and felsic crystalline bedrock aquifers. Water from wells in mafic crystalline bedrock had the lowest radon concentrations. Samples from wells completed in saprolite overlying a felsic crystalline-rock aquifer had higher radon concentrations than the concentrations in wells in the mafic crystalline-rock aquifer. Although general patterns were evident from analysis of the radon data, the range in concentrations in each of these areas was also large. This variability is probably because of the fact that, although radon concentration is directly related to the mineral content of the various rock types, it is the variation in the minor amounts of uranium within

those rocks that controls the actual concentration. This variability is typically not known or mapped on a scale useful for predicting radon. The majority of the wells sampled in this area had radon concentrations between the proposed MCL of 300 pCi/L and the AMCL of 4,000 pCi/L.

In general, concentrations of nitrate, pesticides, and VOCs were related to land-use factors. The concentrations of radon were related to bedrock type and the specific lithology. Although most of these samples were from domestic supply or monitor wells and are not subject to drinking-water standards, the results of the analyses were compared to the USEPA MCLs. None of the 47 pesticides or 59 VOCs analyzed exceeded the MCLs where those constituents were sampled. Nearly 91 percent of the wells sampled exceeded the proposed MCL for radon, but only 13 percent of those wells exceeded the AMCL.

Because the well networks were not initially designed for regional analysis of water quality in the PAS, there are some limitations in interpretation of the results. A lack of sampling density in the southern part of the PAS is a particular weakness. Another issue is the lack of variation in potential explanatory variables, such as land use or aquifer type. Additional sampling representative of specific land-use/aquifer-type combinations would provide a better opportunity to determine statistical relations between water quality and explanatory variables. Resampling of all constituents in selected areas to provide consistent detection limits would enhance the ability to assess the quality of water in the PAS.

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