Relations of Nonpoint-Source Nitrate and Atrazine Concentrations in the High Plains Aquifer to Selected Explanatory Variables in Six Nebraska Study Areas

By A.D. DRULINER, H.H. CHEN, and T.S. MCGRATH

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BRUCE BABBITT, Secretary

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Gordon P. Eaton, Director

For addtional information write to:

District Chief
U.S. Geological Survey
Room 406, Federal Building
100 Centennial Mall North
Lincoln, Nebraska 68508

Copies of this report can be purchased from:

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CONTENTS

FIGURES

FIGURES—Continued

TABLES

CONVERSION FACTORS

Multiply	By	To obtain
inch	25.4	millimeter
foot	0.3048	meter
mile	1.609	kilometer
square mile	2.590	square kilometer
acre	4,047	square meter
acre	0.4047	square hectometer
pound	453.6	gram
ton (short)	0.9072	megagram
pound per acre	1.121	kilogram per hectare
foot per day	0.3048	meter per day
foot per mile	0.1894	meter per kilometer
gallon per minute	0.06309	liter per second
acre-foot	1,233	cubic meter
foot squared per day	0.09290	meter squared per day

Temperature can be converted to degrees Celsius (^oC) or degrees Fahrenheit (^oF) by the equations:

$$^oC = 5/9\ (^oF - 32)$$
$$^oF = 9/5\ (^oC) + 32.$$

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Abstract

Statistical techniques were used to relate nonpoint-source ground-water contamination by nitrate and atrazine to a variety of explanatory variables for six study areas in Nebraska. Water samples collected from 268 wells in 12 counties from 1984 through 1987 were analyzed for nitrate concentrations; samples from 210 of the wells were analyzed for atrazine. A number of hydrochemical, climatic, hydrologic, soil, and land-use explanatory variables, which were believed to affect the contamination of ground water by agricultural chemicals, were identified and quantified for each of the 268 wells.

Scatter plots, simple correlation, multiple regression, and logistic regression methods were used to determine which explanatory variables were statistically related to ground-water concentrations of nitrate and atrazine. Regression models predicting nitrate and atrazine concentrations were produced that explained from about 50 to 68 percent of the variation in the dependent variables. Explanatory variables used to predict nitrate concentrations were: the number of registered irrigation wells within a 1.7-mile radius of the sampled well, average soil permeability in a 60-inch profile, average hydraulic conductivity of the unsaturated zone, specific conductance, and median completion date of registered irrigation wells within a 1-mile radius. Explanatory variables used to predict atrazine concentrations were: nitrate concentration, the depth to water, average hydraulic conductivity of both the unsaturated and saturated zones, specific conductance, average percentage of clay in a 60-inch soil profile, gradient of the potentiometric surface, ground-water temperature, number of registered irrigation wells within a 1.7-mile radius of the sampled well, average hydraulic conductivity of the saturated zone, and average soil permeability of a 60-inch profile.

Logistic regression models predicted the probability of detectable concentrations of atrazine and correctly identified the presence or absence of atrazine about 80 percent of the time. The explanatory variables used by these models were: specific conductance, gradient of the potentiometric surface, transmissivity of the unsaturated zone, depth to water, average percentage of clay in a 60-inch soil, log of the well depth, and number of registered irrigation wells within a 1.7-mile radius of the sampled well.

Geographic-information-system methods were used to produce maps predicting nitrate and atrazine concentrations in ground water for one study area using selected regression and logistic models. The results of this study indicate that multiple regression techniques coupled with geographic information systems can be an effective means of identifying areas of potential ground-water contamination by nitrate and atrazine. The models produced by these methods are area specific and are functions of the apparent dominant processes in the study areas and the data that were available to quantify them.

INTRODUCTION

Farmers in Nebraska, like most throughout the Nation, rely on fertilizers and pesticides to maximize crop yields and sustain productivity over time. Inorganic fertilizers such as nitrogen and broadleaf herbicides such as atrazine have been applied annually to large areas within Nebraska for more than 30 years. In 1989, Nebraska farmers applied an estimated 662 tons of nitrogen fertilizers (as nitrogen) (Nebraska Department of Agriculture, 1985–1989). In 1987, an estimated 28.6 million pounds of herbicide active ingredients were applied in Nebraska (Baker and others, 1990), an 18-percent increase over 1982 estimates (Johnson and Kamble, 1984). Planted acreages declined by about 13 percent during the same period.

Nebraskans rely almost exclusively on ground water as their sole source of drinking water (Steele, 1988), and degradation of this resource by agricultural chemicals or other contaminants is a major concern. In some areas of the State during the last two decades, concentrations of nitrate (as nitrogen) in ground water have exceeded the U.S. Environmental Protection Agency's (USEPA) (1991) Maximum Contaminant Level (MCL) of 10 mg/L (milligrams per liter) for finished public drinking-water supplies, and trace amounts of atrazine have been detected frequently in relatively broad spatial distributions (Exner and Spalding, 1990). This pattern of nitrate concentrations is believed to be a classic example of nonpoint-source contamination (Gormly and Spalding, 1979).

Not all areas of Nebraska in which these agricultural chemicals are regularly used exhibit ground-water contamination (Chen and Druliner, 1987). This variability suggests that one or more combinations of physical factors may be affecting the transport of these chemical contaminants into the ground water. An improved understanding of the relations of these contaminants to quantifiable physical factors could offer more insight to the mechanisms that affect agricultural chemical contamination and aid in the determination of areas that are particularly susceptible to this form of contamination. In 1984, the Toxic Substances Hydrology Program of the U.S. Geological Survey (USGS) began 14 reconnaissance studies to determine the effects that human activities at the land surface have had on regional ground-water quality (Helsel and Ragone, 1984). The Nebraska study (Chen and Druliner, 1987) investigated the presence of selected agricultural chemicals in ground water in portions of the High Plains aquifer and was one of seven studies selected for a more intensive second phase of activity.

Purpose and Scope

This report describes the results of the final phase of the Nebraska study. The purpose of this phase was to determine to what extent the local climatic, hydrologic, soil, and land-use conditions might be related to the variations in nitrate and atrazine concentrations in the ground water, to better define their relations to agricultural contaminants, and to provide techniques that may be used to delineate areas of potential ground-water contamination by selected agricultural chemicals. The report contains a listing of all investigated explanatory variables and a more detailed discussion of selected variables that are believed to affect nitrate and atrazine concentrations in ground water. Finally, the report describes examples of several mathematical models that determine the potential for ground-water contamination by nitrate and atrazine.

Acknowledgments

The authors are grateful to numerous individuals and organizations who facilitated the data collection and statistical interpretation. We acknowledge members of the U.S. Soil Conservation Service's National Laboratory, who were available for consultation and who provided soil analyses, and numerous landowners and tenants who permitted access to their wells and supplied cropping, irrigation, and chemical-use data. Also we are grateful to the Water Center of the University of Nebraska, who provided us with their compilation of regional ground-water-quality data, collected by a variety of local sources.

DESCRIPTION OF STUDY AREAS

The study encompasses 12 counties in Nebraska that are located in the unglaciated portion of the High Plains section of the Great Plains physiographic province (Fenneman, 1946). The counties are grouped into six study areas. The study areas contain from one to three counties each, and all are underlain by the High Plains aquifer. The location and identification numbers of the six study areas are shown in figure 1.

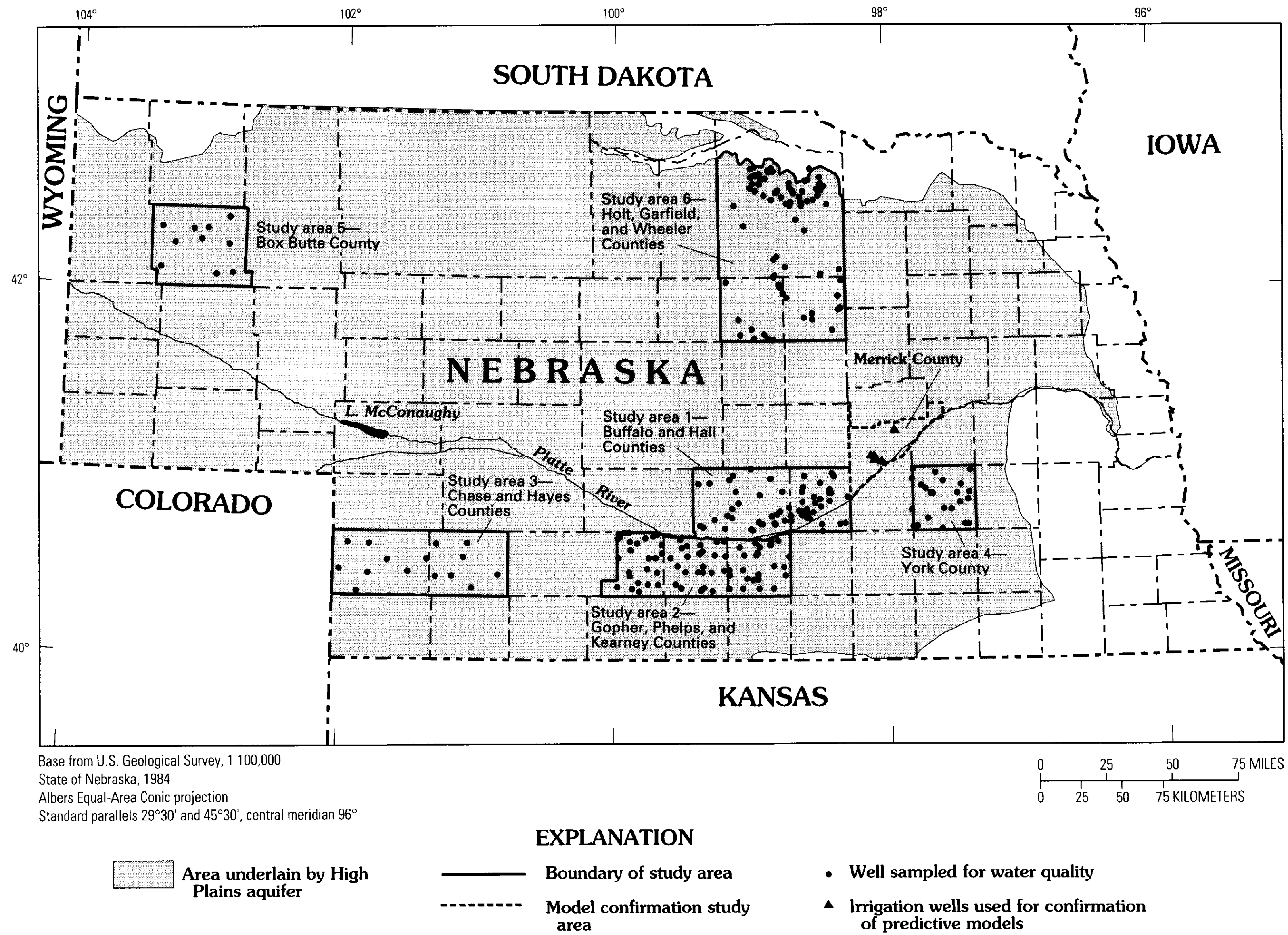

Figure 1. Extent of the High Plains aquifer in Nebraska, location of the six study areas, wells sampled for water quality, and irrigation wells used for confirmation of predictive models.

These areas were selected to provide a wide range of climatic, hydrologic, soil, and land-use conditions in addition to targeting some areas of existing and potential ground-water contamination by agricultural chemicals. A brief description of the hydrology, soil, and land use in the study areas follows; a more detailed description is found in Chen and Druliner (1987).

Hydrology

The High Plains aquifer is largely unconfined and in Nebraska consists mostly of calcareous silt, sand, and sandstone with some zones of coarse sand and gravel of Tertiary age. In some areas clay, silt, and sand of Quaternary age overlie and are hydraulically connected to the Tertiary deposits. Sediments that make up the High Plains aquifer in Nebraska vary in thickness from a few feet to about 800 feet and are underlain by relatively impermeable clay in most areas and some chalk deposits of Cretaceous age in study area 4. The hydrologic characteristics of the High Plains aquifer vary among and within study areas; however, some generalizations can be made. The direction of ground-water flow tends to follow the surface topography and is generally to the east. The median gradient of the potentiometric surface in the six study areas (based on water-level measurements in 268 wells) is 8.3 feet per mile. The hydraulic conductivity of the aquifer is variable depending on the degree of calcareous cementation of the Tertiary deposits and the abundance of Quaternary clay and silt deposits. The range of hydraulic conductivity as estimated from grain-size analysis (Piskin, 1974) of driller's logs for the 268 wells used in this study was 2 to 245 feet per day, with a median of 59 feet per day. The estimated ground-water-flow velocities varied from less than 0.01 foot per day to more than 10 feet per day, with a median velocity of 0.42 foot per day at the 268 wells.

Recharge throughout most of the High Plains aquifer in the six study areas occurs chiefly from precipitation. Additional recharge is provided by seasonal irrigation return flows and leakage from streams, rivers, and irrigation canals. Discharge from the aquifer in the six study areas occurs primarily through irrigation-well pumpage, with secondary losses from evapotranspiration in lowland areas and through seepage into streams, lakes, and canals during periods of low flow.

Soils

Soils are a function of the local topography, geology, climate, and biology of the areas in which they are formed. Given the wide areal distribution of the study areas, it follows that the soils associated with these areas are quite variable. The following discussion of soils was derived largely from the University of Nebraska (1990) and is intended only to provide a very general description of the dominant soils in the study areas.

In study areas 1 and 2, the principal soil types were formed on loess and Platte River alluvial deposits. The loess-derived soils were formed on the uplands and are mostly silty soils with moderate permeability. The Coly-Uly-Holdrege and Holdrege-Uly-Coly soil associations predominate in the uplands. Bottom lands and terrace deposits along the Platte River have produced silty and sandy soils that are exemplified by the Hord-Hall soil association and the Gibbon-Gothenburg-Platte soil association, respectively. Additionally, south of and parallel to the Platte River in study area 2 is a band of loamy and sandy soils formed on eolian sand deposits. The Kenesaw-Hersh and Hersh-Valentine soil associations are common in this area.

Two general types of soils are found in study area 3. The Kuma-Keith-Colby soil association is typical of the silty soils formed on loess deposits in the southeastern half of study area 3. The Valent-Woodly-Jayem and the Jayem-Sarben-Valent soil associations are representative of the sandy loamy to sandy soils that were formed on eolian sand deposits in the western part of study area 3.

Most of study area 4 is upland, and the soils are mostly silty with clayey subsoils that formed on loess deposits. The Hastings-Fillmore soil association is dominant in study area 4. The Hobbs-Hord soil association consists of well-drained, fine silt and is typical of soils formed in alluvium and bottom lands.

Study area 5 is the farthest west and has the most arid climate of the six areas. The loamy- to coarse-loamy and sandy soils are formed here on upland loess, weathered sandstone, or eolian deposits. The Keith-Alliance-Rosebud and Busher-Sarben-Tassel soil associations are the most common loamy soils within study area 5. The Valent and Valentine-Wildhorse soil associations are typical of the sandy soils produced on eolian deposits in the uplands and valleys, respectively, within study area 5.

Study area 6 is the largest of the study areas. Stabilized Quaternary sand dunes occupy the southern half of this study area and have developed predominately well-drained, sandy soils such as the Els-Valentine-Ipage soil association. In the northern part of the area, six fine- to coarse-loamy soils have formed on upland and terrace deposits and are typified by the Jansen-O'Neill-Meadin and the Dunday-Pivot soil associations.

Land Use

Land use in the study areas is almost exclusively agricultural. In 1989, about 45 percent of the 6,279,804 acres in the combined study areas was cropland, with most of the balance in pasture and rangeland. Corn was the principal crop in four of the six areas and was the second most common crop in the remaining two areas (table 1). A total of 1,464,000 acres in the study areas was planted to corn in 1989, which represents about 52 percent of the total cropland in the study areas. About 762,000 acres in the six study areas were planted to wheat and hay, the next most common crop types in 1989, for a total of about 27 percent of the combined cropland. Wheat and hay tend to dominate the more northern study areas (areas 5 and 6). The remaining 20 percent of the cropland was planted in soybeans, sorghum, and assorted small-grain crops. Figure 2 shows a generally increasing trend in the number of acres planted to corn and soybeans and a decreasing trend in the numbers of acres planted to wheat and sorghum during 1955–89 within

Table 1. Agricultural and irrigation data for the six study areas in Nebraska
[Data from Nebraska Department of Agriculture, 1989, except as noted]

Study area (fig. 1)	Land area (acres)	Percent that is cropland	Percent of cropland that is irrigated	Number of registered irrigation wells[1]	Estimated irrigation water used during 1985[2] (acre-feet)	Major crops grown (percent of cropland each occupied in 1989)
1	948,594	59	84	6,580	384,490	Corn (64), hay (12), soybeans (10), sorghum (5), wheat (4).
2	972,325	67	72	4,047	466,840	Corn (68), wheat (9), soybeans (8), sorghum (8), hay (6).
3	1,028,371	35	77	1,712	274,810	Corn (47), wheat (32), hay (8), sorghum (6), dry beans (5).
4	368,486	80	59	2,651	174,560	Corn (64), sorghum (19), soybeans (13).
5	689,280	33	72	946	164,410	Wheat (44), corn (21), dry beans (14), beets (9), hay (9).
6	2,272,748	30	42	3,031	283,060	Hay (58), corn (35), soybeans (4).
Total	**6,279,804**					

[1]From Ellis, Steele, and Wigley (1990). [2]From Steele (1988).

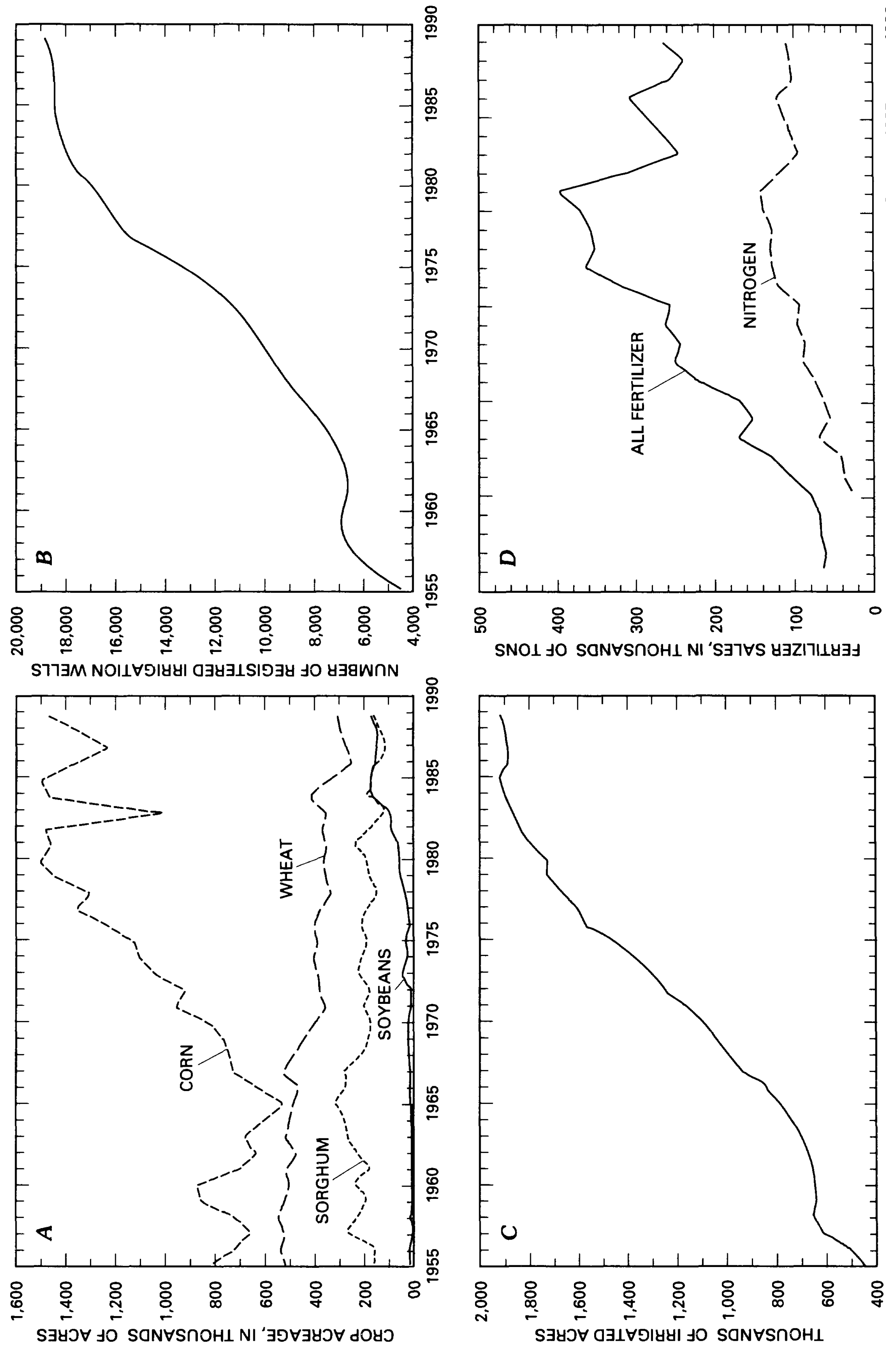

Figure 2. Trends in (*A*) crop acreages, (*B*) number of registered irrigation wells, (*C*) number of irrigated acres, and (*D*) fertilizer sales for six study areas (data from Nebraska Department of Agriculture and Inspection 1957–1984; Nebraska Department of Agriculture, 1985–1989).

the study areas. Corn has been a dominant crop throughout that 34-year period. The fluctuations of the curve for acres planted to corn during the 1980's may be the result of Federal agriculture programs, such as the Payment-In-Kind program, that provided benefits to farmers who reduced their corn acreages.

Water Use

Irrigation is the dominant consumptive water use in Nebraska and accounted for about 93 percent of the State's consumptive water use in 1985 (Steele, 1988). About 65 percent of the cropland in the study areas is irrigated, and corn is the primary recipient, with about 93 percent of the corn acreages in the study areas receiving irrigation water in 1989. Just under 2 million acre-feet of irrigation water were applied to the study areas in 1985. Ground water comprised most of the irrigation water, with about 19,000 active registered irrigation wells identified in the study areas (Ellis and others, 1990). Figure 2 (*B* and *C*) shows the trend in the number of registered irrigation wells and irrigated acres from 1955 through 1989 in the study areas.

Agricultural Chemical Use

The use of inorganic fertilizers and pesticides to maintain high crop yields is a common practice throughout the study areas, especially for irrigated corn production. Nitrogen is the dominant component in most fertilizers applied in the study areas and commonly is applied in the form of anhydrous ammonia, which usually is injected into the soil prior to planting. Other forms of nitrogen used in fertilizers in the study areas include ammonium nitrate, ammonium sulfate, urea, and solution of urea-ammonium nitrate in water. Under oxidizing conditions, these compounds tend to be converted to nitrate, which is anionic and quite mobile in water. The rates of nitrogen application for cornfields varies considerably depending on the type of corn that is to be grown, the yield goal for the field, and the amount of nitrogen present in samples of shallow soil and ground water that will be used for irrigation. The Cooperative Extension Service of the University of Nebraska (University of Nebraska, 1979) commonly recommends from 60 to 280 pounds of nitrogen per acre on fields in which corn is being grown for grain in an area of low soil nitrogen content (about 50 pounds per acre). The use of nitrogen fertilizers in the six study areas increased from 1960 through the early 1980's to a maximum of about 147,000 tons of nitrogen per year (fig. 2*D*). Through the remainder of the 1980's, nitrogen fertilizer use was fairly steady at a rate of slightly more than 100,000 tons of nitrogen per year.

Pesticides also frequently are used on cropland in the study areas and across the State, especially on cornfields. Approximately 81 percent of the more than 23 million pounds of active herbicide ingredients and 96 percent of the 4.8 million pounds of active insecticide ingredients used in the State in 1987 were applied to cornfields (Baker and others, 1990). Atrazine, which is a broadleaf triazine herbicide used with corn, accounted for slightly more than one-half (13.4 million pounds) of the active herbicide ingredients applied in Nebraska in 1987.

Atrazine commonly is used as a preplant, or preemergent herbicide, and less often as a post-emergent herbicide on cornfields to control broadleaf and grassy weeds. It frequently is applied by incorporation into the top few inches of soil at planting time in the mid- to late-spring. Supplementary applications may be made later in the summer by combining atrazine with irrigation water and applying the mixture through overhead sprinkler irrigation systems or by a single lay-by cultivation. Recommended atrazine application amounts vary from 2 pounds of active ingredients per acre for sandy loam soils to 3 pounds per acre for silty-clay loam soils (University of Nebraska, 1985a). Atrazine also can be used in concert with other herbicides, a practice that is becoming more common as concern over ground-water contamination with atrazine increases. These combinations frequently use 1 to 1.5 pounds of atrazine per acre.

During the 5-year period from 1982 to 1987, the estimated herbicide use for corn crops in the State increased by 25 percent, whereas the number of acres of corn treated with herbicides decreased by 13 percent (Johnson and Kamble, 1984; Baker and others, 1990). Thus, it appears that the net use of herbicides on corn per treated acre has been increasing during this time period.

METHODS

The approach of the study was fourfold. First, a variety of potential explanatory variables was identified, and data describing these variables were compiled for selected wells in each of the study areas.

Second, ground-water samples were collected and analyzed for nitrate and triazine herbicides over a period of several years in the study areas. Third, a series of predictive statistical models was generated using the water-quality and explanatory data. Finally, the accuracy of selected statistical models was checked by making predictions in a different area and comparing observed water-quality concentrations with predicted values. Additional model confirmation was done by graphically comparing areas of predicted contamination with areas of observed ground-water contamination in study area 1 from data sources not used to generate the models.

Identification of Explanatory Variables

Initially, 21 explanatory variables were identified and used for preliminary analyses of predictive methodologies in the reconnaissance phase of this study (Chen and Druliner, 1987). The number of variables was expanded during the final phase of the study to include a total of 75 possible explanatory variables that were grouped into the following categories: hydrochemical, climatic, hydrologic, soil, land use, and geomorphic. These variables are listed in table 2.

Values for the hydrochemical explanatory variables were obtained from both onsite measurements and laboratory analyses of ground-water samples collected during the course of this study from 268 wells located within the six study areas.

Values for the climatic explanatory variables for each of the 268 wells were obtained by interpolating data from 20 weather data-collection sites located in or adjacent to the six study areas and operated by the Center for Agricultural Meteorology and Climatology, Institute of Agriculture and Natural Resources, University of Nebraska-Lincoln. An inverse distance-decay function was used to produce distance-weighted average values for the 29 climatic variables for each of the 268 wells using the three weather data-collection sites closest to each well. This approach proved acceptable for study areas with several weather data-collection sites nearby but produced a very narrow range of values for study areas 5 and 6 because they each had a single nearby weather data-collection site that dominated the distance-weighted averages.

Hydrologic explanatory variables were described by data obtained from a variety of sources. The bulk of this information came from driller's logs for irrigation and municipal wells from which ground-water samples were collected and from geologic test holes and driller's logs for other wells near many of the 268 wells. The average screened well depth was determined by calculating the median depth of all screened intervals in each well. The average hydraulic conductivity was estimated from individual driller's logs using sediment grain-size analyses (Piskin, 1974). The hydraulic gradient and depth to water (assumed to be the depth to the water table) for each of the 268 wells were determined using spring and fall water-level data from a water-level measurement program conducted by the Conservation and Survey Division of the University of Nebraska and the USGS. Ground-water-flow velocities were estimated at each well using the average hydraulic conductivity, the hydraulic gradient, and an estimated porosity of 20 percent (Freeze and Cherry, 1979). The specific capacity for registered irrigation wells was determined by dividing the estimated discharge rates by drawdown values that were obtained from the Nebraska Department of Water Resources (NDWR) irrigation-well registration data. The specific-yield values were obtained from estimates made by Pettijohn and Chen (1983).

Soil explanatory variables were obtained from U.S. Department of Agriculture, Soil Conservation Service, county soil survey reports (see references) for the fields adjacent to each of the 12 counties and from the U.S. Department of Agricultural, Soil Conservation Service, National Soils Laboratory's computerized data set. The dominant soil association(s) for the fields adjacent to each of the 268 wells were determined using the county soil maps. Depth-integrated averages for the 60-inch profile were generated for each of the soil variables listed in table 2. The National Soils Laboratory's computerized data set was used to supply soils data for soil types or associations that had missing measurements in the county soil survey reports.

Land-use data were derived from onsite observations and discussions with the landowners or operators at the time of ground-water sample collection and from the NDWR computerized irrigation-well registration data. Landowners and operators were asked to supply information about crop types; the history, methods, and rates of chemical application; irrigation methods, dates, and amounts; tillage techniques and frequency; locations of current and abandoned stock yards, septic tanks, and chemical storage areas; and well depth and date of well installation and initiation of irrigation for fields serviced by or other land

Table 2. Explanatory variables that may affect nitrate and atrazine concentrations in ground water in the six study areas in Nebraska

Hydrochemical

Specific conductance
pH
Temperature

Climatic

Maximum air temperature:
- April through June
- July through September
- Growing season[1]
- Dormant season[2]

Average air temperature:
- April through June
- July through September
- Growing season[1]
- Dormant season[2]
- Annual

Predicted evapotranspiration:
- April through June
- July through September
- Growing season[1]
- Dormant season[2]
- Annual

Actual evapotranspiration:
- April through June
- July through September
- Growing season[1]
- Dormant season[2]
- Annual

Precipitation:
- April through June
- July through September
- Growing season[1]
- Dormant season[2]
- Annual

Effective precipitation:
- April through June
- July through September
- Growing season[1]
- Dormant season[2]
- Annual

Hydrologic

Average screened well depth
Average hydraulic conductivity:
- Unsaturated zone
- Saturated zone
- Unsaturated and saturated zones

Transmissivity:
- Unsaturated zone
- Saturated zone
- Unsaturated and saturated zones

Thickness of clay deposits:
- Unsaturated zone
- Saturated zone
- Unsaturated and saturated zones

Gradient of potentiometric surface
Depth to water
Ground-water flow rate
Specific capacity
Specific yield
Well depth

Soil

Available water content
Moist bulk density
Organic matter content
Percent clay
Permeability
pH
Slope

Land use

Acres serviced by sampled well
Type of tillage used on field serviced by the sampled well
Number of cultivations of field serviced by the sampled well
Rate of nitrogen application on fields serviced by sampled well
Rate of atrazine application on fields serviced by sampled well
Atrazine application date
Date of first irrigation application of sampled year

Land use—Continued

Number of irrigated acres within 1.7-mile radius of the sampled well
Median number of irrigated acres in all fields within 4-mile radius of the sampled well
Number of registered irrigation wells within the same 1-square-mile section as the sampled well
Number of registered irrigation wells within 1.7-mile radius of the sampled well
Estimated gallons per minute pumped from the sampled well
Median gallons per minute pumped from registered irrigation wells within a 1.7-mile radius of the sampled well
Year the well was drilled
Median year of installation of all registered irrigation wells within 1-mile radius of the sampled well
Median year of installation of all registered irrigation wells within a 1.7-mile radius of the sampled well
Median depth of all registered irrigation wells within a 1.7-mile radius of the sampled well

Geomorphic

Drainage area
Drainage density
Physiographic area

[1]Growing season is from April through September.
[2]Dormant season is from October through March.

adjacent to each of the 268 wells from which water samples were collected.

The irrigation-well registration data set maintained by the NDWR provided additional land-use and irrigation data. These data included the locations of all active registered irrigation wells, the number of acres irrigated by each well, the well depth, drilling date, the discharge rate, and water levels before and after a limited aquifer-test period. These data were used in geographic-information-system (GIS) computer programs to generate median values for various irrigation-related land-use variables for radii around each of the wells from which ground-water samples were collected. This permitted a potentially more representative assignment of values to selected land-use variables for each of the 268 wells. Several geomorphic variables were examined in the reconnaissance phase of the study. Most were found to explain little variation in the concentrations of nitrate and atrazine in the ground water. However, physiographic area was examined during the final phase of the study. The physiographic-area variable represents a combination of the soil type and topographic location of the sampled wells, and is divided into three categories: bottom lands, terraces, and uplands.

Water-Quality Data Collection

Water samples were collected from 268 wells in the study areas during 1984 through 1987. The locations of the sampled wells are shown in figure 1. In 1984, 82 wells were identified in the six study areas for the reconnaissance phase of the study. Subsequent ground-water sample collection occurred only in study areas 1, 2, 4, and 6. Water samples were collected once from each well. All 268 water samples were analyzed for nitrite plus nitrate concentrations (hereinafter referred to as nitrate), and 210 samples were analyzed for triazine herbicides, of which atrazine is the most commonly used. Triazine herbicides were selected because they are the most commonly used pesticides within the study areas and tend to have the longest half-lives of the more commonly used herbicides (Chen and Druliner, 1987).

Well Selection

Only water wells that were screened in the High Plains aquifer were used for collection of ground-water samples. Sampling areas were selected to provide the best areal distribution while yielding a representative coverage of the dominant agricultural land uses present in each study area. Estimated hydraulic conductivity, well depth, depth to water, and soil type also were considered in the selection of the study areas to provide a wide range of variation in these variables. Once target areas for ground-water samples were identified, available wells within each target area were randomly selected. At this point, well owners were contacted and interviewed by telephone to determine if the selected well was available for sampling, if a driller's log and details of the well's completion were available, what type of chemical and irrigation practices had taken place in the vicinity of the well, and if any possible point sources of nitrogen and pesticides might be present at that well. The final selection of each well was made onsite just prior to sampling to see if other conditions might exist that would compromise the integrity of the water sample.

A total of 222 irrigation, 21 domestic, 21 stock, and 4 municipal wells were selected for water-quality sampling during the course of the study. A variety of these wells was used for sample collection during the reconnaissance phase of the study, with the emphasis on registered irrigation wells during the final phase of the study. This emphasis was maintained because registered irrigation wells were the only available wells located within cropped agricultural settings that had driller's logs and well-completion data on file.

Water samples were collected from eight additional registered irrigation wells in 1988 in Merrick County, in the valley of the Platte River. These additional wells were selected randomly from nearly 3,900 registered irrigation wells in the county for model confirmation. Confirmational sites were selected in Merrick County because it is an area of intensely irrigated agriculture similar to study area 1 but was not sampled during the initial portion of the study.

Sampling Protocol

All ground-water samples from the study areas were collected between July and early September. Samples were collected from irrigation, municipal, and stock wells only after the wells had been pumped continuously for several hours to several days to obtain water samples representative of aquifer conditions. Water was collected from private domestic wells only after the pressure tank had been drained and the pump had been engaged for about 10 minutes. The water samples were collected from the nearest access point to the pump in each case and before water-treatment systems, such as water softening or other chemical injection. No samples were collected from overhead sprinkler irrigation systems that were actively injecting nitrogen or pesticides into the water. Additionally, such systems were not sampled if chemical injections had been made prior to the sampling visit during that same irrigation season.

Hydrochemical variables, which consisted of specific conductance, pH, and temperature, were measured for all water samples after the well was purged and prior to the filling of the sample bottles. Samples for nitrate analyses were collected, filtered through a 0.45-micron filter into a 250-milliliter polypropylene bottle, and preserved with mercuric chloride. Ground-water samples for pesticide analyses were collected in 1-liter, pre-baked, glass bottles with polytetrafluoroethylene-lined plastic tops following three rinses of the bottle with sample water. All sample bottles were placed immediately in ice chests and kept at 4 °C until they were transferred to laboratory refrigerators. Within 1 week of sample collection, the water samples were packaged in coolers with sufficient ice to maintain a constant 4 °C temperature and sent by 2-day mail to the analyzing laboratories.

Laboratory Analyses and Detection Limits

All water samples were analyzed for dissolved nitrite plus nitrate by the USGS National Water-Quality Laboratory (NWQL) in Arvada, Colorado, using the cadmium reduction method (Fishman and Friedman, 1989).

Two hundred and ten ground-water samples were analyzed by two laboratories for triazine herbicides that included atrazine, cyanazine, prometon, propazine, and simazine. The NWQL analyzed 71 samples collected in 1984 and 1986. The method used by the NWQL employed a methylene chloride extraction followed by gas-chromatographic separation with nitrogen-phosphorus detection (Wershaw and others, 1987). The identification of all triazine herbicides was confirmed through chromatographic separation on a separate column. The minimum reporting limit for atrazine by the NWQL at that time was 0.1 µg/L (microgram per liter), and the minimum quantitative limit was about 0.03 µg/L (Ralph White, NWQL, oral commun., 1985). In some water samples atrazine was determined to be present but in concentrations too small for the NWQL to accurately estimate (below the minimum quantification limit). Confirmed atrazine detections in this category were considered qualitative and were assigned concentrations of 0.02 µg/L by the authors for the purpose of including these data in evaluating relations to selected explanatory variables.

The remaining 139 water samples were analyzed for triazine herbicides during 1985 and 1987 by the Analytical Laboratory of the Department of Microbiology and Environmental Health (DMEH) at Colorado State University in Fort Collins, Colorado, which is a U.S. Environmental Protection Agency (USEPA) contract laboratory. The DMEH laboratory used similar analytical procedures for these analyses as described by Wershaw and others (1987). The minimum quantitative detection limit for atrazine was about 0.04 µg/L. DMEH also reported the presence of confirmed atrazine peaks on chromatograms in which the concentrations were below their capability to accurately quantify. Atrazine detections in this category also were considered qualitative and were assigned a concentration of 0.03 µg/L by the authors, which was a reasonable approximation of the DMEH's minimum qualitative detection limit (John Tessari, DMEH, written commun., 1985).

The eight confirmational water-quality samples collected in Merrick County were analyzed for nitrate concentrations by the NWQL and for atrazine by Harris Environmental Technologies[1], Inc., of Lincoln, Nebraska. Harris Environmental Technologies used the same method of atrazine determination as described by Wershaw and others (1987). The minimum quantitative detection limit for atrazine was 0.01 µg/L.

Quality Control and Quality Assurance

Bottles used for sample collection and the mercuric chloride used for nitrate preservation were subject to quality control by the NWQL. The quality-assurance program of the NWQL includes participation in USGS and USEPA interlaboratory evaluations and submission of blind standard-reference water samples into the NWQL analytical sequence (Friedman and Fishman, 1982; Jones, 1987).

About 5 percent of the water samples analyzed for atrazine were quality-assurance samples and were comprised of a combination of blind duplicate and spiked samples that were submitted to the principal

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[1]Any use of trade, product, or firm names is for descriptive purposes only and does not constitute endorsement by the U.S. Government.

contract laboratory analyzing the water samples. Replicate samples were collected seconds after and under the same conditions as the original sample, and were submitted to the analyzing laboratory with false identification numbers. Six of these replicate samples also were analyzed for herbicide concentrations by the University of Iowa Hygienic Laboratory in Iowa City, Iowa. A series of spiked pesticide samples prepared by the NWQL were rebottled, relabeled, and included in shipments of environmental water samples to the analyzing contract laboratory. Comparisons were made among the actual spiked concentrations, the NWQL's analyses of the sample, and the contract laboratory's analysis of the sample.

Modeling Techniques

Ground-water concentrations of nitrate and atrazine were related to corresponding values for each of the explanatory variables through several techniques. The first technique consisted of simply producing scatter plots of the dependent variables with each of the explanatory variables. This provided an approximate determination of the type of relation that existed between the variables, the distribution of the values, and an estimate of the variation of each variable. Next, correlation coefficients were generated for each of the dependent and explanatory variable pairs. Various transformations of the explanatory variables were produced, and the transformed variables were plotted again and correlated to the dependent variables to see if the linear relation was improved.

Multiple linear regression techniques as described by Minitab, Inc. (1989) and the SAS Institute, Inc. (1990) were used to develop regression models with nitrate and atrazine concentrations as the dependent variables. Regression procedures used included stepwise, stepwise forward, stepwise backward, best regression, maximum R, and R-squared. In applying the Minitab, Inc. (1989) stepwise regression computation, a minimum F-statistic of 1.8 was specified to determine which explanatory variables would remain in the models, although all models containing explanatory variables with F-statistics less than 3.8 (and with T-ratio less than 1.9) later were rejected. The maximum R and R-squared techniques in SAS Institute, Inc. (1990) were designed to maximize the coefficient-of-determination values (percentage of explained variation) for each model by stepwise selection of explanatory variables or by considering all combinations of explanatory variables, respectively. Plots of the residuals versus the predicted values were produced for each model, and the Lilliefors test (1967) was used to determine whether the residuals were nonnormally distributed at the 95-percent confidence level.

Logistic regression methods (SAS Institute, Inc., 1990) also were used. These methods utilized discrete values for the dependent variable, such as the presence or absence of an analyte at the (qualitative) analytical detection limit, and both discrete and continuous explanatory variables. Through a maximum-likelihood methodology, this technique produced multiple regression models that predicted the probability of the presence or absence of the dependent variable at the specified detection value. This approach was particularly useful when working with explanatory variables that contain very limited ranges, as is the case with many of the climatic and soil variables. The method also permitted greater utilization of data representing wells in which atrazine was not detected. The goodness of fit for logistic models was determined by comparing the percentages of correct and incorrect predictions rather than through coefficients of determination.

The logistic regression methods were used to predict the probability of detection of atrazine in ground-water samples. The nitrate data contained few nondetection values and lended themselves better to more traditional regression techniques. All atrazine concentrations greater than the minimum (qualitative) analytical detection limit of 0.02 μg/L were classified as events, and all concentrations less than that value were classified as nonevents. This binary version of the dependent variable was used to generate the models presented later in this report. Models were considered acceptable if they represented logically plausible relations with the explanatory variables and if the probability of exceeding the Chi-square statistic was less than 0.05 for each explanatory variable included in the model.

Model Confirmation

Selected models were confirmed using two separate approaches. First, eight registered irrigation wells were selected randomly for water-quality sampling from registered wells in Merrick County, which is immediately to the northeast of study area 1 (fig. 1). Ancillary data describing the explanatory variables for the eight wells were used by selected models to predict nitrate and atrazine concentrations and probability of atrazine detections in the ground water. The predicted concentrations and probabilities of detections were compared to observed concentrations and frequencies of detection.

The second means of confirmation utilized ground-water nitrate and atrazine data sets for study area 1 that were compiled by researchers from the University of Nebraska, Lincoln. Because the ancillary data describing many of the explanatory variables used in the models to be verified were not available for the wells in this data set, only a visual comparison was made between the spatial distributions of observed ground-water concentrations of nitrate and atrazine and spatial distributions of predicted concentrations and probabilities of atrazine detections.

RESULTS OF WATER-QUALITY ANALYSES AND COMPARISONS AMONG STUDY AREAS

The results of the nitrate and atrazine analyses of water samples collected from 1984 through 1987 are published in annual data reports (U.S. Geological Survey, 1985–88) and are summarized in table 3. The median ground-water concentration of nitrate for the 268 analyses was 4.5 mg/L. Concentrations of nitrate ranged from less than 0.05 to 57 mg/L. Twenty-eight percent of these samples had nitrate concentrations that exceeded the USEPA's MCL of 10 mg/L for nitrate in finished public drinking-water supplies (U.S. Environmental Protection Agency, 1991).

Study area 1 had the largest median ground-water concentration of nitrate (9.8 mg/L) of the six study areas; this was followed by study area 6 with a median concentration of 6.4 mg/L. Results of the Kruskal-Wallis test (Kruskal and Wallis, 1952)

Table 3. Statistical summary of results of nitrate and atrazine analyses of ground-water samples for the six study areas in Nebraska, 1984–87

Study area (fig. 1)	Number of analyses	Minimum	Maximum	Twenty-fifth percentile	Median	Seventy-fifth percentile	Number of concentrations exceeding 10 milligrams per liter
			Nitrate concentration, in milligrams per liter				
1	65	<0.05	57	1.4	9.8	25	32
2	78	.1	32	2.3	3.8	7.6	10
3	15	1.7	4.0	2.0	2.3	2.9	0
4	24	<.05	28	4.0	4.8	6.3	2
5	11	2.4	13	2.5	3.3	5.7	1
6	75	.1	51	1.6	6.4	18	30
All	**268**	**<.05**	**57**	**2.2**	**4.5**	**11**	**75**
Study area (fig. 1)	**Number of analyses**	**Minimum**	**Maximum**	**Twenty-fifth percentile**	**Median**	**Seventy-fifth percentile**	**Number of detections**
			Atrazine concentration, in micrograms per liter				
1	57	<0.02	3.5	<0.01	0.14	0.87	36
2	72	<.02	.98	<.02	<.02	.07	31
3	9	<.02	<.02	<.02	<.02	<.02	0
4	20	<.02	2.2	<.02	<.02	<.02	4
5	10	<.02	.70	<.02	<.02	<.02	2
6	42	<.02	1.8	<.02	.03	.10	25
All	**210**	**<.02**	**3.5**	**<.02**	**<.02**	**.16**	**98**

showed that the median nitrate concentrations of ground-water samples from all the study areas were not the same at the 95-percent confidence level. The Mann-Whitney test (Mann and Whitney, 1947) then was used to statistically compare the median concentrations of nitrate in the six study areas, and the concentration in study area 1 was found to be significantly larger at the 95-percent confidence level than the median concentrations for each of the other study areas with the exception of study area 6. Study area 3 had a median nitrate concentration significantly smaller than the other five areas.

Forty-seven percent of the 210 ground-water samples analyzed for atrazine contained detectable concentrations. Most water samples containing detectable concentrations of atrazine were near the analytical quantitative detection limits of 0.02 to 0.04 µg/L. The maximum concentration of atrazine detected was 3.5 µg/L. This sample and one other contained atrazine concentrations in excess of the USEPA's MCL of 3.0 µg/L for finished public drinking-water supplies (U.S. Environmental Protection Agency, 1991).

Study areas 1 and 6 displayed the largest median ground-water concentrations of atrazine, with values of 0.14 and 0.03 µg/L, respectively. The median ground-water concentration of atrazine was less than 0.02 µg/L for the remaining four study areas. The Kruskal-Wallis test showed that the median atrazine concentrations for ground-water samples from all of the study areas were not the same at the 95-percent confidence level. The Mann-Whitney test indicated that the median atrazine concentration in study area 1 was significantly larger at the 95-percent confidence level than the median concentrations of the other five study areas and that the median atrazine concentration from water samples in study area 6 was significantly larger than the medians from study areas 3, 4, and 5.

Comparison of the quality-assurance data for atrazine showed that the DMEH Laboratory was performing acceptably. The duplicate samples analyzed for atrazine showed that the precision of the DMEH Laboratory was within about 20 percent. Comparison of duplicate water samples analyzed for atrazine at both the DMEH Laboratory and the NWQL were in general agreement. The analysis of samples of known concentration prepared by the NWQL and submitted as disguised environmental samples to the DMEH Laboratory showed that the DMEH Laboratory correctly identified the presence of atrazine in all samples that were known to contain atrazine. These analyses also showed that the DMEH Laboratory tended to underestimate the known atrazine concentrations. Since the samples of known atrazine concentration were not reanalyzed by the NWQL in the same timeframe as the DMEH Laboratory, it is not known if the smaller atrazine concentrations detected by the DMEH Laboratory were actually the result of analytical bias or atrazine degradation.

RELATIONS OF NITRATE AND ATRAZINE CONCENTRATIONS TO SELECTED EXPLANATORY VARIABLES

The first method used to explore relations among the explanatory variables and concentrations of nitrate and atrazine was inspection of Lowess smoothed (Cleveland, 1979) scatter plots of explanatory variables and the dependent variables (nitrate and atrazine concentrations). The Lowess smoothed plots enhance the perception of possible relations between the variables. Scatter plots of selected explanatory variables and nitrate and atrazine concentrations in ground water from the six study areas, correlation coefficients, and discussion of apparent relations follow. As reported by Chen and Druliner (1987), nitrate and atrazine concentrations in ground water from the six study areas were closely related. The Pearson correlation coefficient (Iman and Conover, 1983) for data collected during this study for the two variables was 0.70. As shown in figure 3, the majority of water samples containing detectable concentrations of atrazine also contained nitrate concentrations greater than 5.0 mg/L. Although the concentrations of the two contaminants varied by several orders of magnitude, 74 percent of the water samples with detectable concentrations of atrazine also contained nitrate concentrations greater than 5.0 mg/L. This suggests that the transport of both contaminants is sensitive to many of the same environmental conditions.

Of the remaining hydrochemical variables, specific conductance demonstrated monotonic relations with both nitrate and atrazine concentrations (fig. 4) and had Spearman's correlation coefficients of 0.47 and 0.48, respectively. The trend exhibited by the Lowess smoothed plots suggests that the nitrate concentration in ground water constitutes a substantial part of the total dissolved constituents and that specific conductance in some of these areas may be a surrogate for nitrate content in the water.

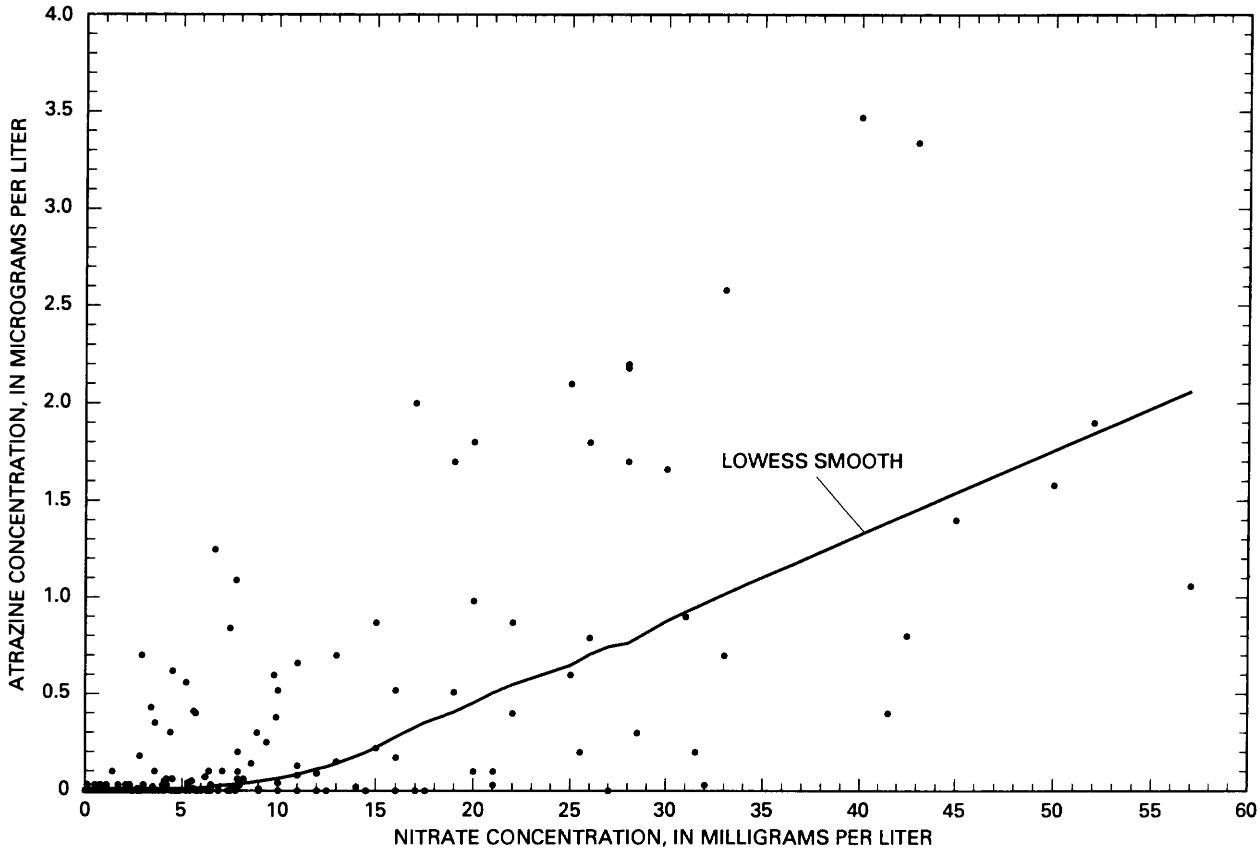


Figure 3. Relation of nitrate to atrazine concentrations in ground-water samples from six study areas in Nebraska, 1984–87.

The majority of climatic variables (table 2) did not show particularly pronounced relations with nitrate and atrazine concentrations when plotted. This probably is due in part to the coarseness of these data when extrapolated from climatic data-collection sites to the sampled wells. Additionally, it seems logical to assume that, with the practice of intensive irrigation, many of the climatic factors have relatively little effect on the potential for ground-water contamination with nitrate and atrazine, especially in the presence of more influential variables. Scatter plots of the relation of nitrate concentrations to evapotranspiration during the growing season, precipitation during the growing season, and annual precipitation are shown in figure 5. As would be expected, ground-water concentrations of nitrate tended to decrease slightly with greater evapotranspiration and to increase with increased amounts of seasonal and annual precipitation. Evapotranspiration may retard the leaching of nitrate through the unsaturated zone by drawing soil moisture upward. Increased amounts of precipitation would be expected to increase the leaching of nitrate into the ground water.

Several hydrologic variables showed discernible relations when plotted with nitrate and atrazine concentrations. The ground-water concentrations of both nitrate and atrazine increased directly with increases in average hydraulic conductivity (fig. 6), showing Spearman's correlation coefficients of 0.46 and 0.52, respectively. The relation with nitrate concentrations has a nearly uniform slope throughout the range of hydraulic-conductivity values encountered in the study areas. The relation with atrazine concentrations shows more sensitivity to hydraulic-conductivity values exceeding about 70 feet per day and reflects, in part, the tendency for atrazine to sorb onto finer materials (Weed Science Society of America, 1983).

Depth to water was inversely related to ground-water concentrations of nitrate and atrazine, with Spearman's correlation coefficients of -0.37 and -0.54, respectively. The plots of depth to water with nitrate and atrazine concentrations (fig. 7) revealed a depth below which ground-water nonpoint-source

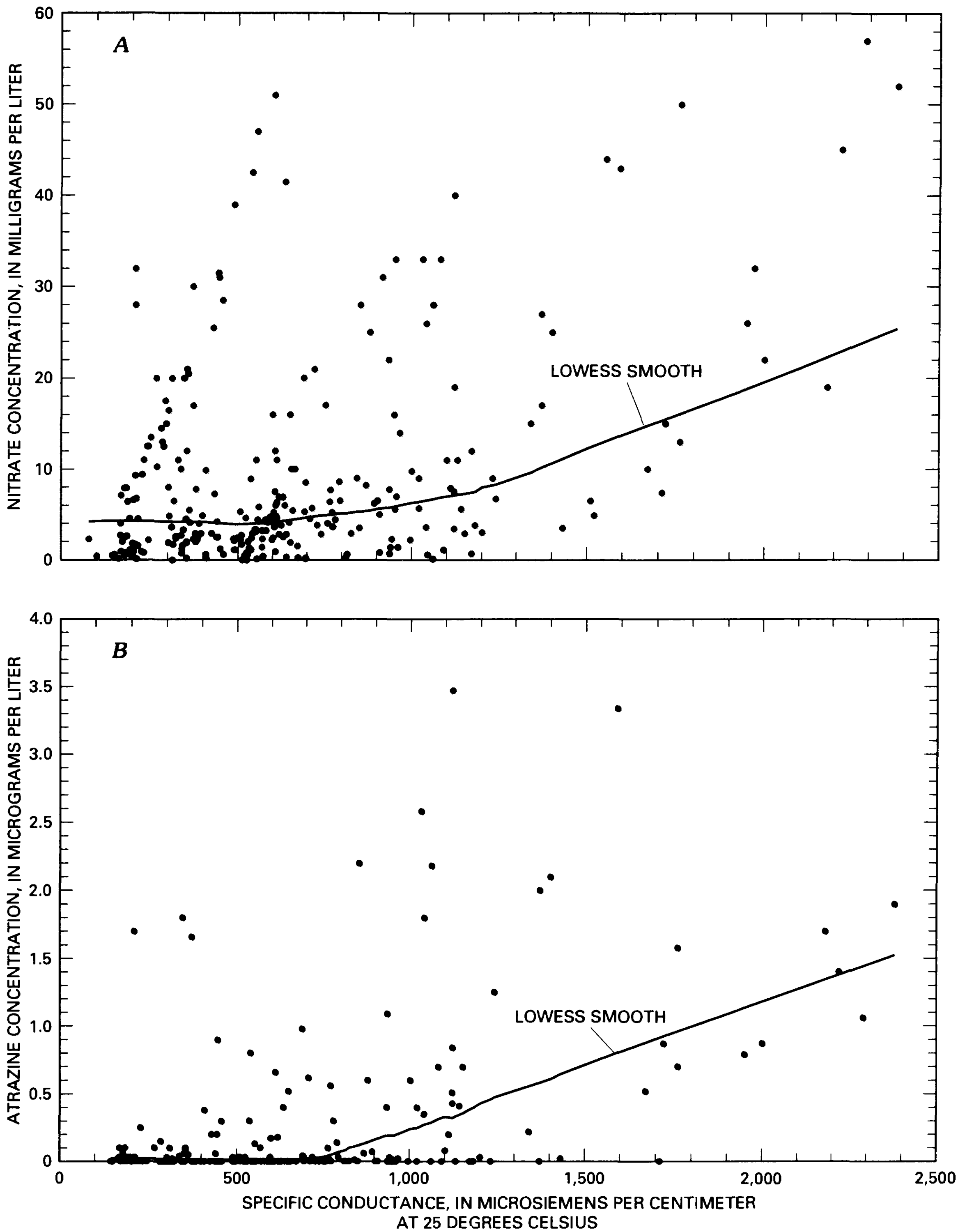


Figure 4. Relation of (*A*) nitrate and (*B*) atrazine concentrations to specific conductance in ground-water samples from six study areas in Nebraska, 1984–87.

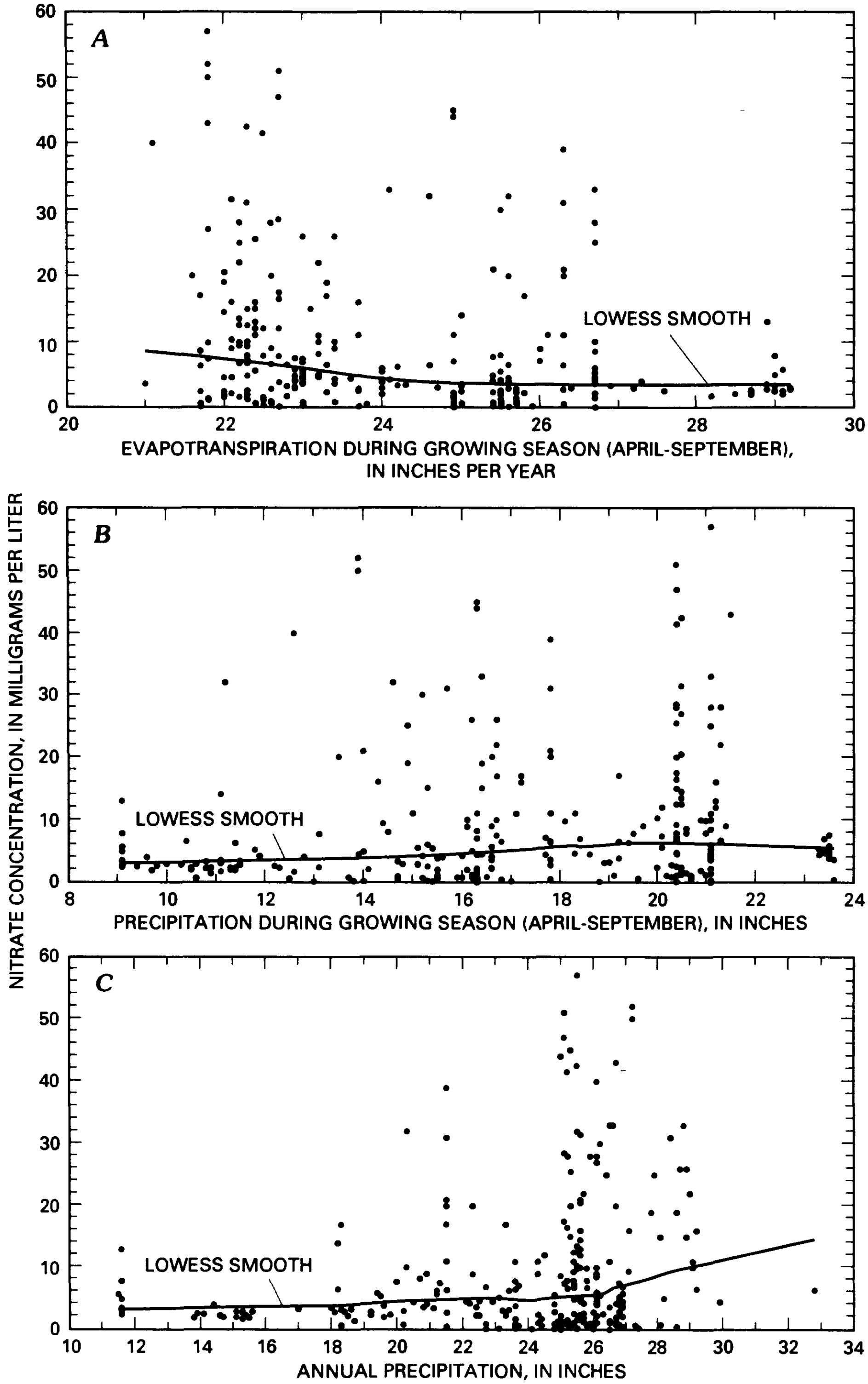


Figure 5. Relation of nitrate concentrations in ground-water samples from six study areas in Nebraska to (*A*) evapotranspiration during the growing season, (*B*) precipitation during growing season, and (*C*) annual precipitation, 1984–87.

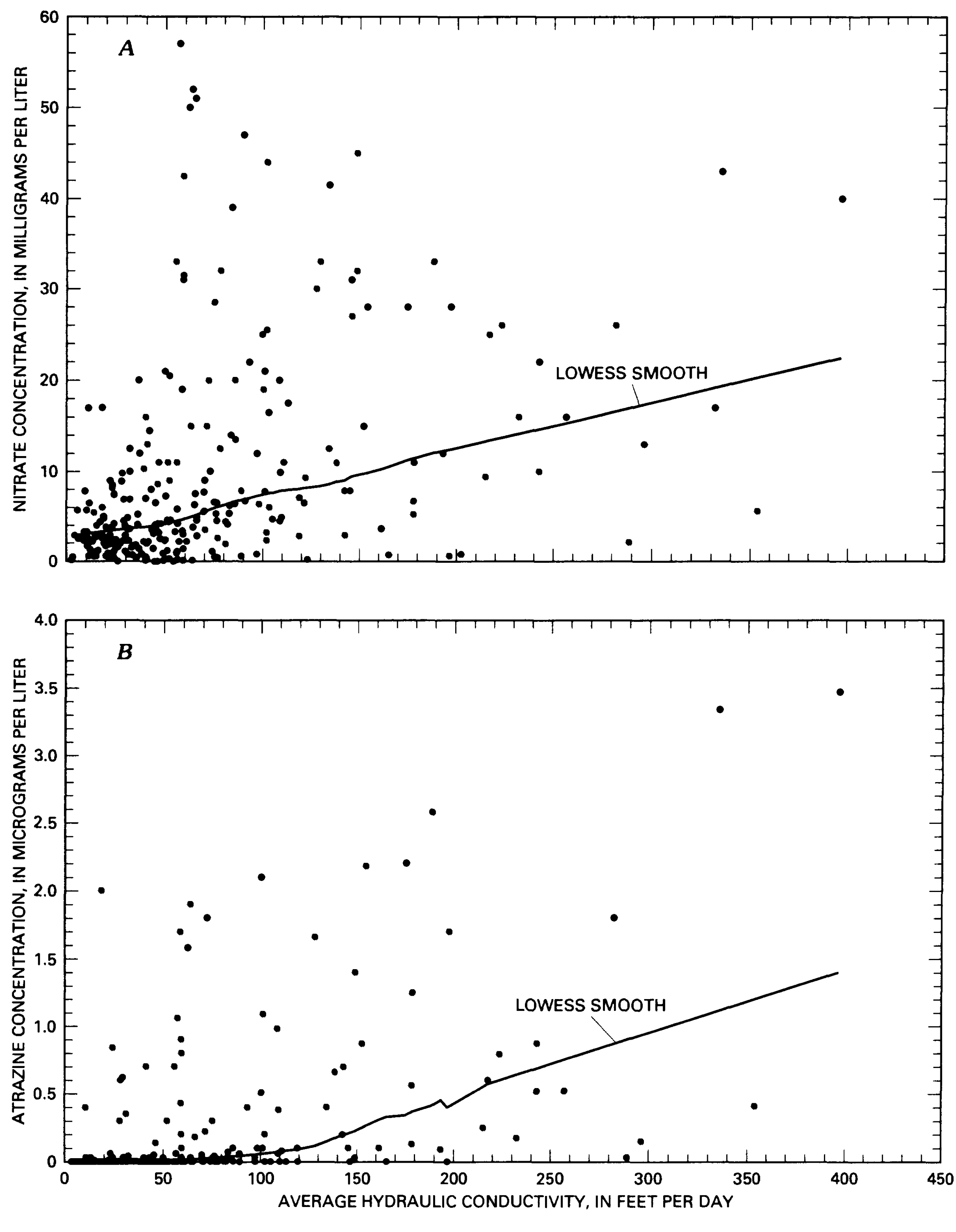


Figure 6. Relation of (A) nitrate and (B) atrazine concentrations in ground-water samples from six study areas in Nebraska to average hydraulic conductivity calculated from driller's logs, 1984–87.

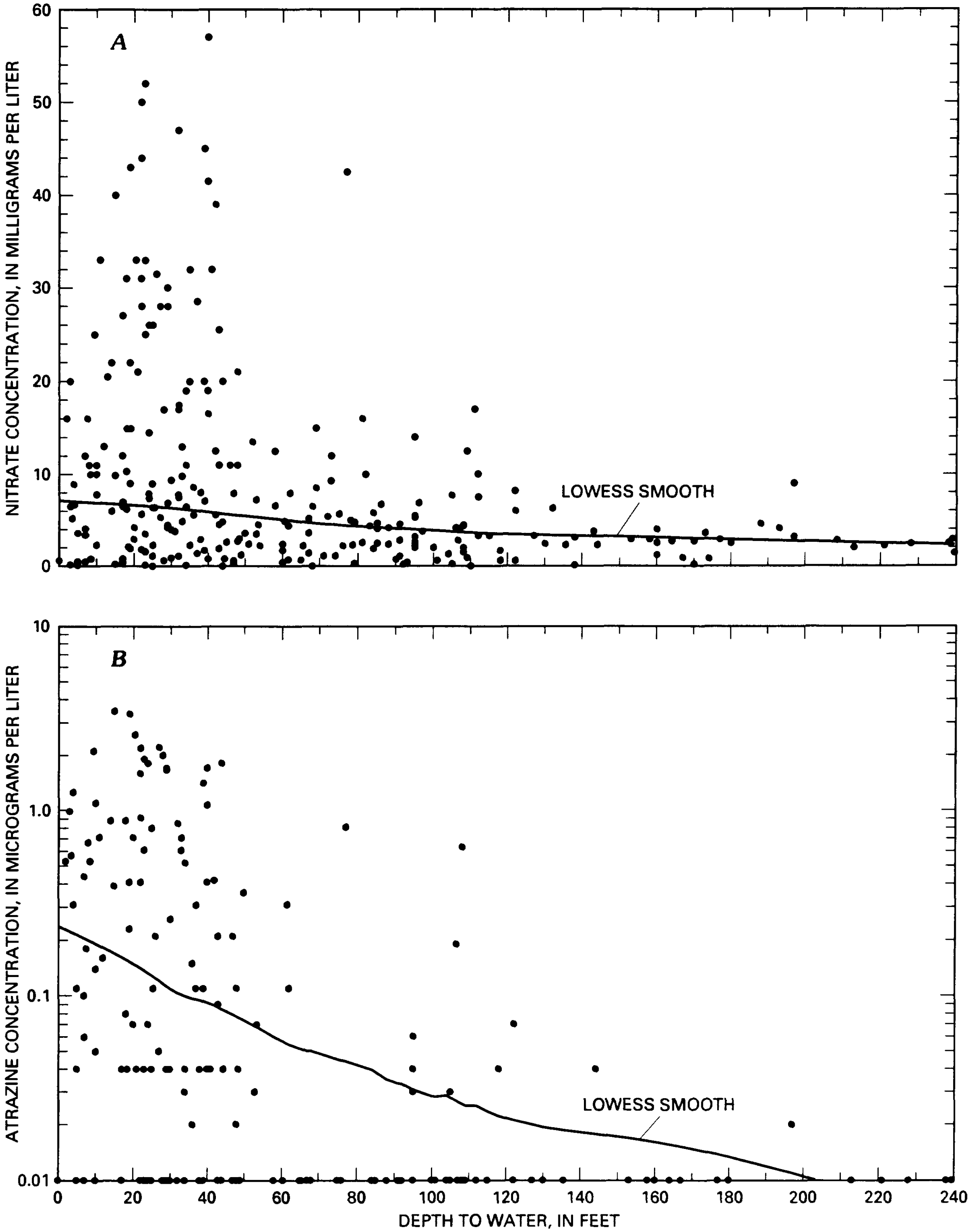


Figure 7. Relation of (*A*) nitrate and (*B*) atrazine concentrations in ground-water samples from six study areas in Nebraska to depth to water, 1984–87.

contamination in the study areas appears less likely. Most of the ground water with nitrate concentrations greater than 10 mg/L was from wells with depths to water of less than 60 feet. Wells sampled with depths to water greater than 60 feet (42 percent of all sampled wells) accounted for only 13 percent of the samples with nitrate concentrations equal to or greater than 10 mg/L. Similarly, detectable concentrations of atrazine rarely were found in water from wells with depths to water greater than 60 feet. In fact, 85 percent of the water samples containing detectable concentrations of atrazine were from wells with depths to water of 50 feet or less (56 percent of all wells from which water samples were analyzed for atrazine). Additionally, all water samples with atrazine concentrations equal to or larger than 1.0 mg/L were from wells with depths to water of less than 50 feet.

The depths of wells from which the water samples were collected also showed inverse relations with concentrations of both nitrate and atrazine (fig. 8), with Spearman's correlation coefficients of -0.49 and -0.54, respectively. About 80 percent of nitrate concentrations greater than 10 mg/L were from wells with depths not exceeding 150 feet (39 percent of all wells in the study). Atrazine concentrations displayed a comparable relation with well depth. More than 65 percent of the water samples with detectable concentrations of atrazine were from wells whose depths were equal to or less than 150 feet (40 percent of all wells from which water samples were analyzed for atrazine).

Soil explanatory variables showed limited associations with ground-water concentrations of nitrate and atrazine. As with the climatic variables, the relatively weak relations are believed to be caused by the coarseness of the soil variable characterization. Most of the soil explanatory variables were quantified from data supplied by county soil survey reports of the immediate area around each sampled well.

Some of the explanatory variables, such as the average percentage of clay in the 60-inch soil profile, showed limited relations when plotted with nitrate and atrazine concentrations (fig. 9). Although the relations suggested by the scatter plots were generally weak, with Spearman's correlation coefficients for nitrate and atrazine concentrations of -0.14 and -0.40, respectively, 71 percent of the water samples with nitrate concentrations equal to or greater than 10 mg/L and 70 percent of the water samples with detectable concentrations of atrazine came from locations in which the dominant soils contained less than 10 percent clay.

A number of land-use explanatory variables showed relations with ground-water concentrations of nitrate and atrazine. The number of active registered irrigation wells within a 1.7-mile radius (9 square miles) of the sampled well showed a positive relation with both nitrate and atrazine concentrations (fig. 10) and Spearman's correlation coefficients of 0.44 and 0.45, respectively. These relations suggest that the potential for ground-water contamination with nitrate and atrazine is greater in areas with more intensive irrigated agriculture, as indicated by the number of active registered irrigation wells. Other land-use variables, such as the number of acres to be irrigated that was estimated when each well was drilled, also showed similar relations to nitrate and atrazine concentrations.

Several additional explanatory variables were derived using the number of active registered irrigation wells within varying radii of the sampled wells. The relations of these derived explanatory variables to nitrate and atrazine concentrations were similar; however, the strength of the relations with nitrate and atrazine concentrations were largest for radii of 1.7 miles. The number of registered irrigation wells is a measure of agricultural intensity. The 1.7-mile radii suggests that wells in areas of similar or larger extent have a greater likelihood of intercepting ground-water flow paths containing nitrate and atrazine contamination than do wells in agricultural areas of smaller extent.

The median completion date of all registered irrigation wells within a 1.7-mile radius of the sampled well displayed a negative relation with both nitrate and atrazine concentrations. Data from the six study areas suggest that wells constructed before the early 1960's have a greater potential for ground-water contamination by nitrate and atrazine. This relation could be the result of two factors. It is possible that improved well construction and placement standards have reduced the likelihood of ground-water contamination. It is more likely, however, that the areas with extensive ground-water development prior to the early 1960's merely have had nitrogen and atrazine applied on associated fields for a longer period of time. This longer history of chemical application may have permitted the contaminants to accumulate in larger concentrations in the ground water with time.

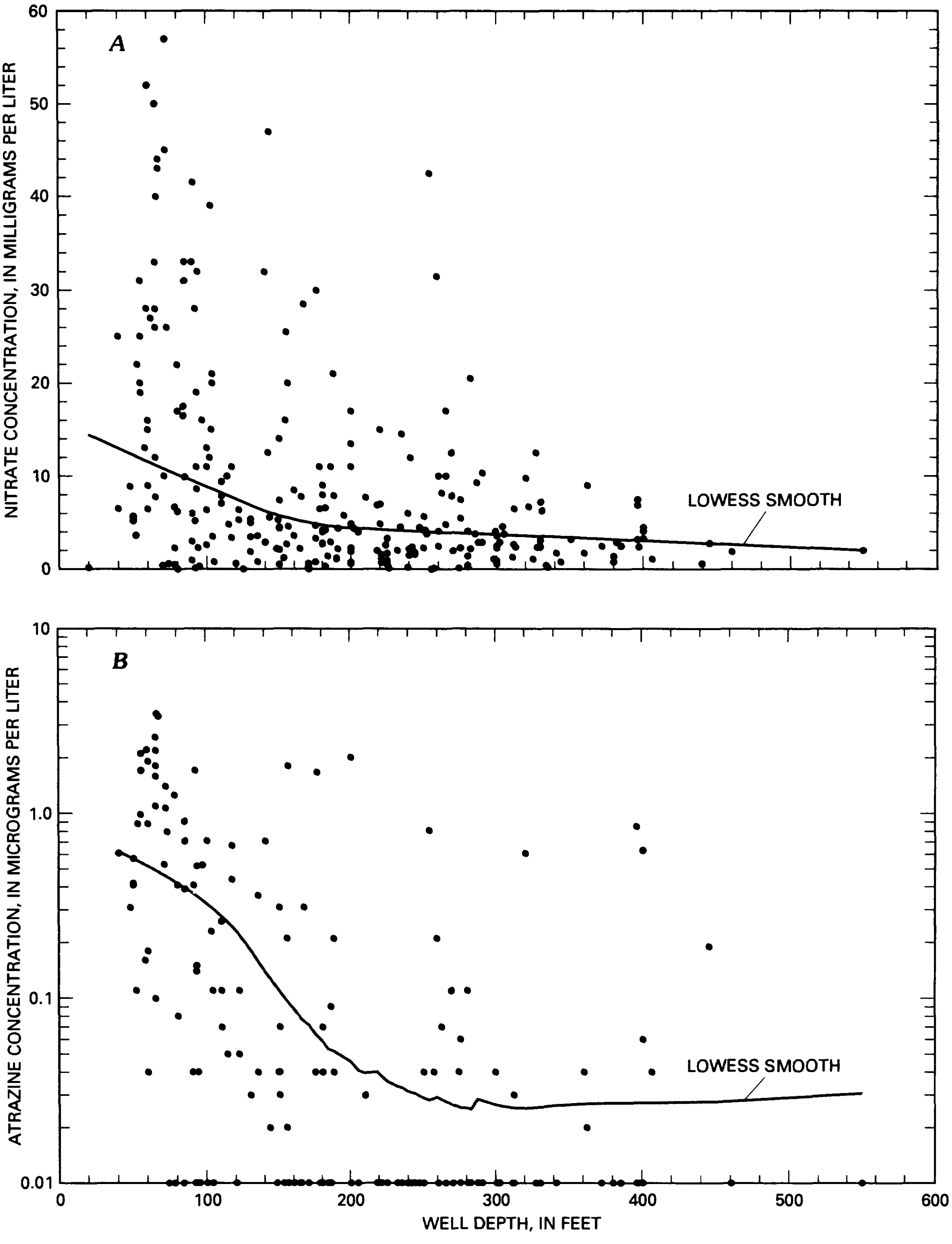


Figure 8. Relation of (*A*) nitrate and (*B*) atrazine concentrations in ground-water samples from six study areas in Nebraska to well depth, 1984–87.

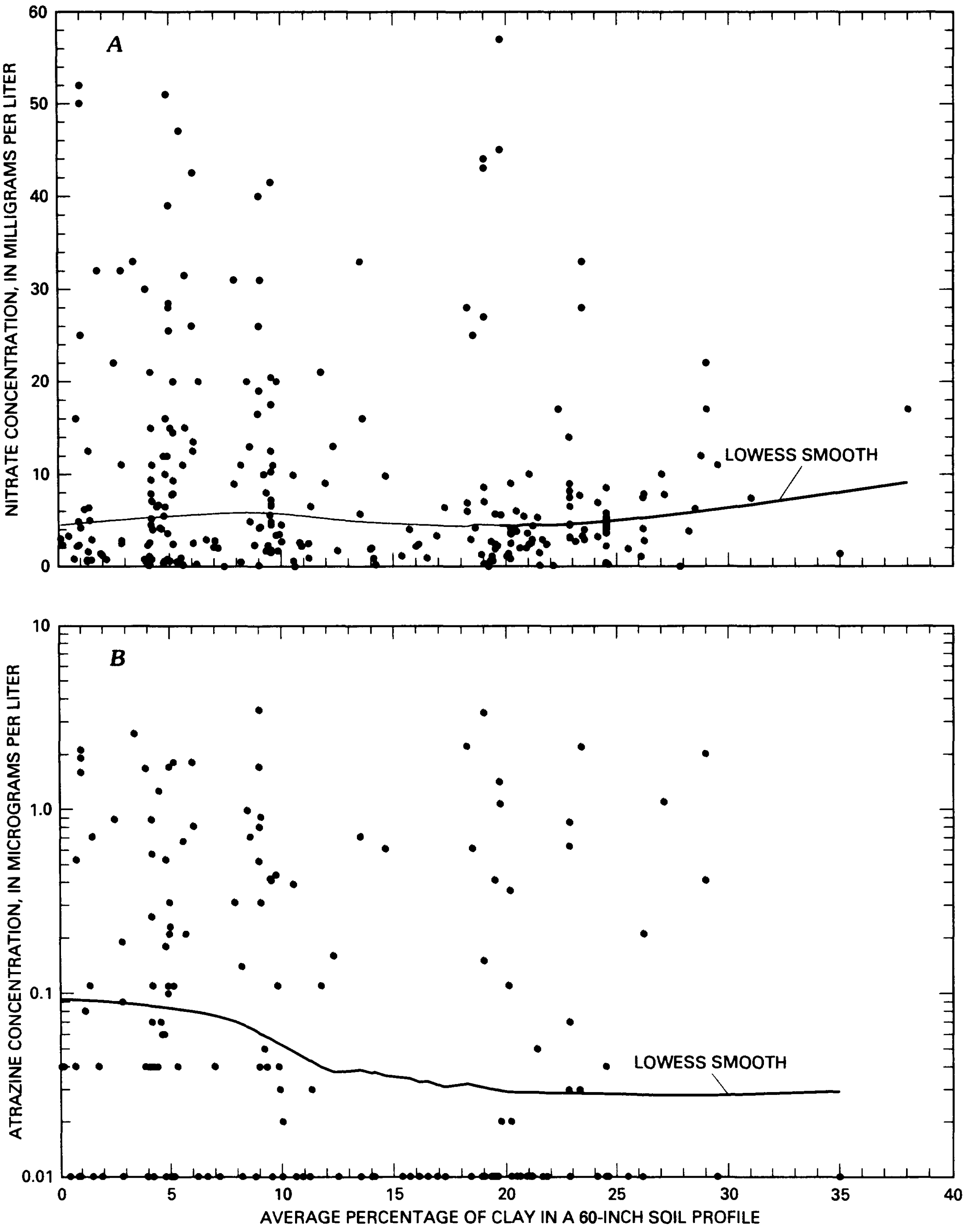


Figure 9. Relation of (*A*) nitrate and (*B*) atrazine concentrations in ground-water samples from six study areas in Nebraska to average percentage of clay in a 60-inch soil profile, 1984–87.

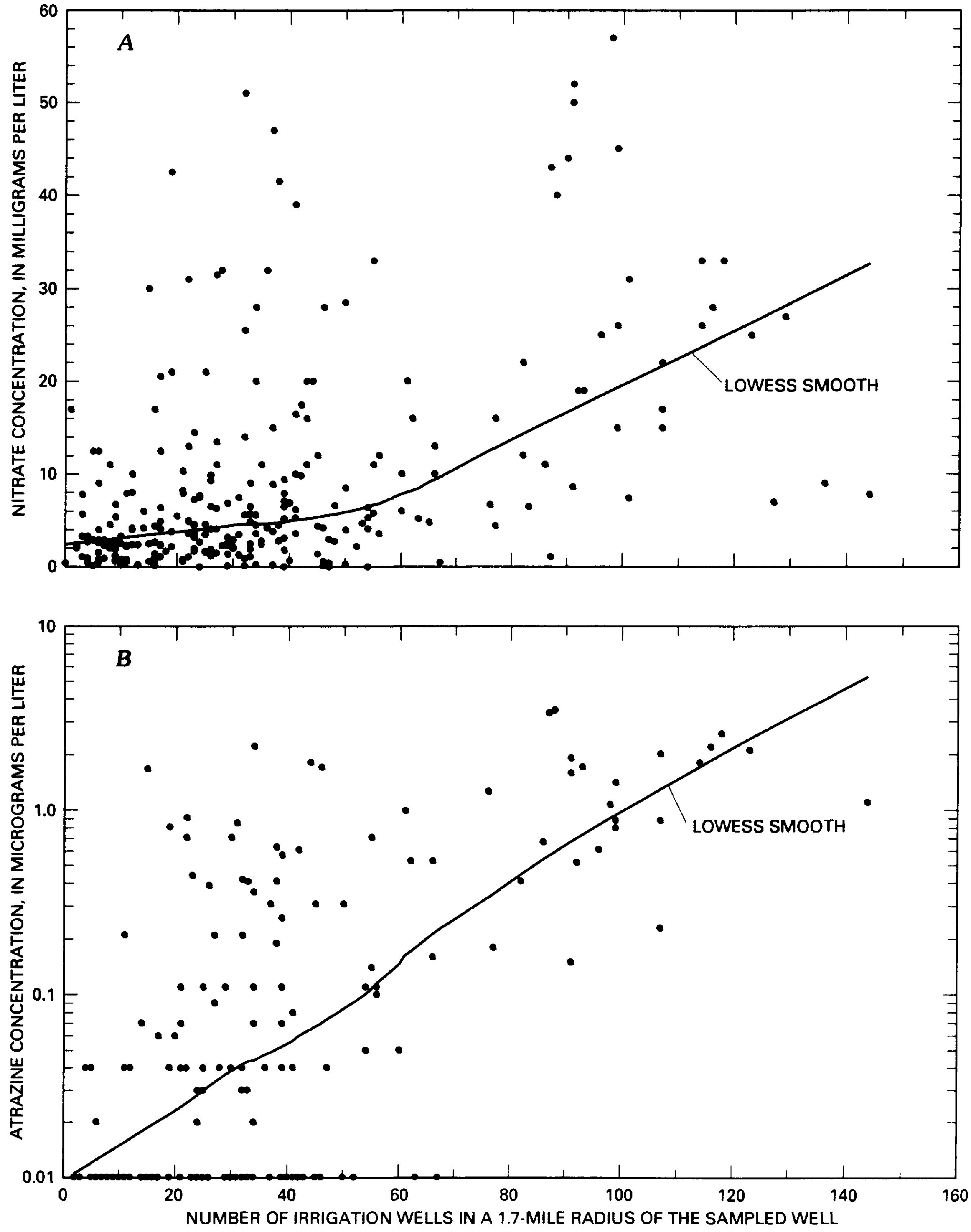


Figure 10. Relation of (A) nitrate and (B) atrazine concentrations in ground-water samples from six study areas in Nebraska to number of registered irrigation wells in a 1.7-mile radius of the sampled well, 1984–87.

SELECTED PREDICTIVE MODELS

Multiple linear regression methods were used to generate models that explained limited amounts of variation in nitrate and atrazine concentrations. The coefficients of determination, which represent the amount of variation in nitrate concentrations that each model was able to explain, ranged from 0.50 to 0.68, and plots of the residuals from these models often displayed nonnormal distributions. Most models contained a mixture of hydrochemical, hydrologic, and land-use variables, whereas few models included climatic variables.

Nitrate Models

Table 4 describes two multiple linear regression models that are representative of the models produced with nitrate concentration as the dependent variable. The first model (model A) was produced using data from all six study areas for each of the sampling years. The second model (model B) was produced using only data from study area 1. The coefficients of determination for the two models were 0.50 and 0.68. The plots of residuals (fig. 11) for both models show that the predictive capability of the models deteriorated with increasing concentrations of nitrate, which is indicated by the increased spread of the residuals from left to right. This nonconstant variance is called heteroscedasticity and is an indication of the reduced reliability of the model.

Two of the same variables are present in both models, and the variables included in each have a logical basis. The presence of specific conductance in both models is reasonable in that it appears to be an indirect measure of the nitrate concentration. Other models, which excluded specific conductance, explained considerably less variation in nitrate concentration. The presence of hydraulic conductivity of the unsaturated zone in both models and average soil permeability of a 60-inch profile, in model A, demonstrate that increased permeability of the shallow materials appears to enhance the likelihood of ground-water contamination by nitrate. Time has been incorporated into model B as the median completion date of registered irrigation wells within a 1-mile radius of the sampled well. This variable suggests that areas with older wells and thus, by implication, longer histories of nitrogen usage, are more likely to have ground water contaminated with nitrogen. Similarly, the inclusion of the number of registered irrigation wells within a 1.7-mile radius of each of the sampled wells used in model A can be interpreted to mean that areas with more irrigation development are more likely to have higher concentrations of nitrate in the ground water. This is reasonable when considering that the sampled wells could intercept water carrying contaminants from adjacent fields upgradient of the sampled well.

Model B in table 4 was produced using data only from study area 1 because those samples had a larger median concentration of nitrate in the ground water than four of the remaining five study areas, as was discussed previously. This model used data from 65 water-quality samples and generated a coefficient of determination of 0.68 using only three explanatory variables: specific conductance, average hydraulic conductivity of the unsaturated zone, and median completion date of all registered irrigation wells within a 1-mile radius of the sampled well. The plot of residuals for model B (fig. 11) approximates a normal distribution and, therefore, provides more assurance as to the validity of the methods used to produce this model. Comparison of the two models demonstrates the general enhancement of predictive power when the modeling techniques were applied to a single area as opposed to a collection of six areas with an associated wider range in natural and land-use characteristics.

Atrazine Models

Multiple Regression Models

Table 5 shows four multiple linear regression models developed using the logarithm (log) of the atrazine concentration as the dependent variable. Before atrazine concentrations were transformed to base^{-10} logs, 0.01 µg/L was added to each atrazine value to prevent the nondetection values from being omitted from the models. The first three models (C–E) were produced using a combined data set for all six study areas. Model F was generated using data from only study area 1 because the median atrazine concentration in water samples from study area 1 was significantly larger than the median concentrations in water samples from the other study areas as determined by the Kruskal-Wallis and Mann-Whitney tests, which were discussed earlier. The models contain from three to six explanatory variables from the hydrochemical, hydrologic, soils, and land-use categories. No climatic

Table 4. Multiple linear regression models with nitrate concentration in ground water as the dependent variable

Explanatory variable	Intercept value or regression coefficient	T-ratio	P-value
Model A—Data from all six Nebraska study areas, all explanatory variables were available for inclusion in the model except pH. **Dependent variable: nitrate, in milligrams per liter** **Number of samples: 263** **Coefficient of determination: 0.50**			
Intercept	-8.44	-6.33	<0.001
Specific conductance, in microsiemens per centimeter at 25 degrees Celsius	.0126	7.95	<.001
Average hydraulic conductivity of the unsaturated zone, in feet per day	.0492	5.51	<.001
Average soil permeability of 60-inch profile, in inches per hour	.685	5.38	<.001
Number of registered irrigation wells within a 1.7-mile radius	.0896	4.24	<.001
Model B—Data from Nebraska study area 1. **Dependent variable: nitrate concentration, in milligrams per liter** **Number of samples: 65** **Coefficient of determination: 0.68**			
Intercept	21.9	2.00	.047
Specific conductance, in microsiemens per centimeter at 25 degrees Celsius	.0149	6.01	<.001
Average hydraulic conductivity of the unsaturated zone, in feet per day	.0804	4.72	<.001
Median completion date of irrigation wells within a 1-mile radius	-.436	1.96	.050

variables explained sufficient variation in atrazine concentrations to be included in the models. The coefficients of determination for the four models ranged from 0.54 to 0.63. Plots of the residuals for only model F approximated a normal distribution at the 95-percent confidence level as determined by the Lilliefors (1967) and Shapiro-Wilk (1965) tests. Plots of the residuals with the log of predicted atrazine concentrations frequently showed the largest variation and, therefore, reduced predictive capability in the center of the plot where atrazine concentrations ranged from -1.5 to -0.5 log units of micrograms per liter (fig. 12).

The explanatory variables used by models C through E are similar. All three models contained nitrate and (or) specific conductance, and all three included depth to water. All the models contained either the average hydraulic conductivity of the saturated and unsaturated zone or just the saturated zone. Two of the models contained a soil explanatory variable, two contained the hydraulic gradient, and two contained the same land-use explanatory variable. The presence of nitrate or specific conductance in the models suggests a strong relation between the presence of atrazine and either nitrate concentration or specific conductance, which is believed to relate to the concentration of nitrate in the ground water. The inclusion of a negative depth-to-water term in all of the regression equations demonstrates the vulnerability of shallow aquifer systems to ground-water

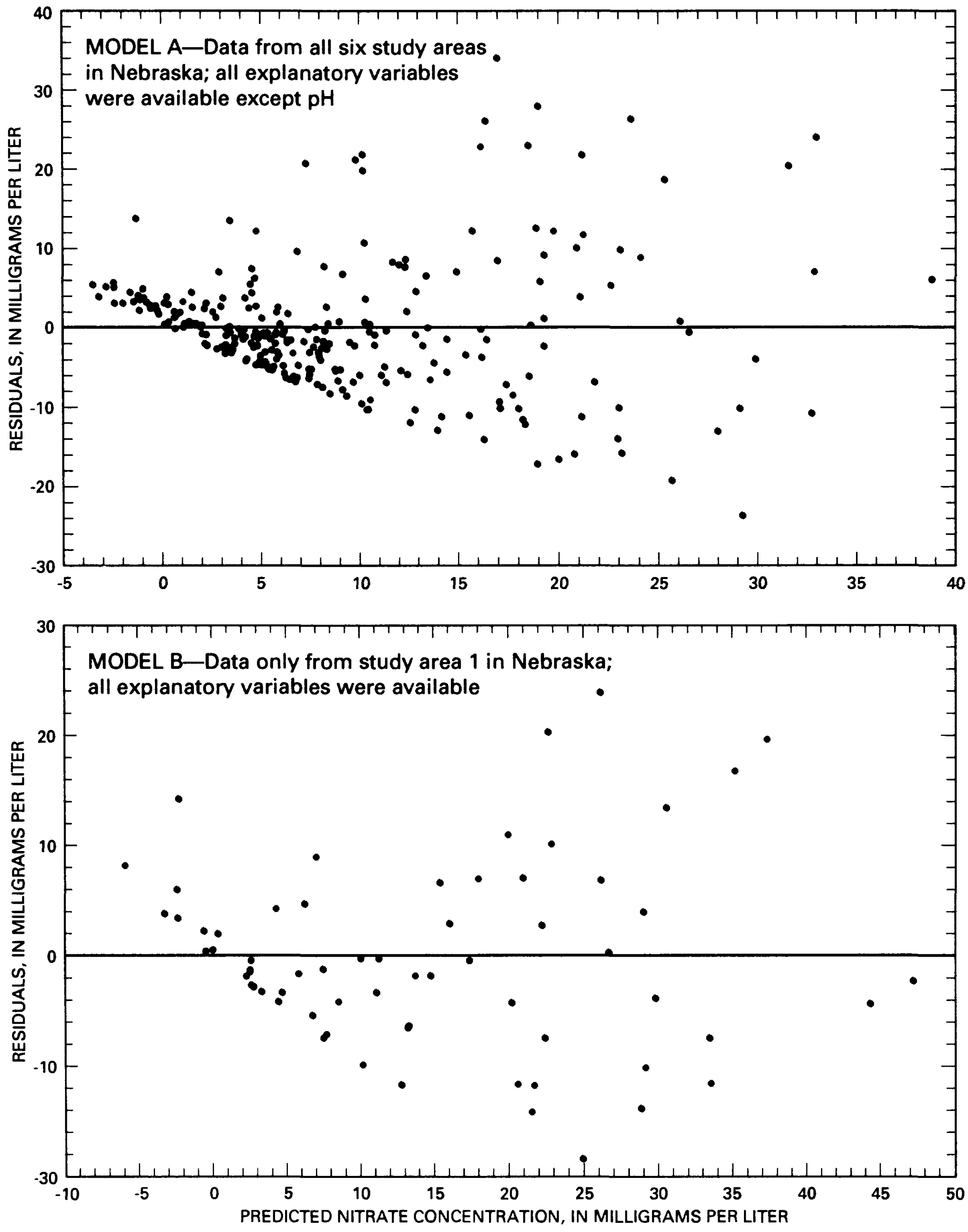


Figure 11. Residual plots for multiple linear regression models predicting nitrate concentrations in ground water.

Table 5. Multiple linear regression models with log of the atrazine concentration as the dependent variable

Explanatory variable	Intercept value or regression coefficient	T-ratio	P-value
Model C—All explanatory variables were available for inclusion in the model; data from all six Nebraska study areas. Dependent variable: log of atrazine concentration, in micrograms per liter Number of samples used: 209 Coefficient of determination: 0.63			
Intercept	-1.74	16.5	<0.001
Nitrate concentration, in milligrams per liter	.03087	7.91	<.001
Specific conductance, in microsiemens per centimeter at 25 degrees Celsius	.000381	4.12	<.001
Average hydraulic conductivity of both the unsaturated and saturated zones, in feet per day	.00250	3.47	.001
Depth to water, in feet	-.00258	3.47	.001
Average percentage of clay in 60-inch soil profile	-.0138	3.14	.002
Model D—All explanatory variables except specific conductance were available for inclusion in the model; data from all six Nebraska study areas. Dependent variable: log of atrazine concentration, in micrograms per liter Number of samples used: 208 Coefficient of determination: 0.62			
Intercept	-2.713	6.36	<.001
Nitrate concentration, in milligrams per liter	.0381	9.76	<.001
Temperature of the ground water, in degrees Celsius	.0850	2.59	.010
Average hydraulic conductivity of both the unsaturated and saturated zones, in feet per day	.00196	3.24	<.001
Gradient of potentiometric surface, in feet per foot	-91.2	3.54	<.001
Depth to water, in feet	-.00324	4.03	<.001
Number of registered irrigation wells within a 1.7-mile radius of the sampled well	.00276	1.91	.058

Table 5. Multiple linear regression models with log of the atrazine concentration as the dependent variable—Continued

Explanatory variable	Intercept value or regression coefficient	T-ratio	P-value
Model E—All explanatory variables except nitrate concentration were available for inclusion in the model; data from all six Nebraska study areas.			
Dependent variable: Log of atrazine concentration, in micrograms per liter			
Number of samples used: 210			
Coefficient of determination: 0.54			
Intercept	-2.26	-12.6	<0.001
Specific conductance, in microsiemens per centimeter at 25 degrees Celsius	.000778	6.12	<.001
Average hydraulic conductivity of the saturated zone, in feet per day	.00259	4.61	<.001
Gradient of potentiometric surface, in feet per foot	-71.9	-2.50	.0133
Depth to water, in feet	-.00192	-2.03	.0432
Average soil permeability of 60-inch profile, in inches per hour	.0531	4.86	<.001
Number of registered irrigation wells within a 1.7-mile radius of the sampled well	.00417	2.19	.0299
Model F—All explanatory variables were available for inclusion in the model; data from study area 1.			
Number of samples used: 57			
Coefficient of determination: 0.61			
Intercept	-1.46	-6.40	<.001
Nitrate concentration, in milligrams per liter	.0359	6.05	<.001
Depth to water, in feet	-.00693	2.52	.015
Number of irrigated acres within a 1.7-mile radius of the sampled well	.0000774	2.02	.048

contamination. The hydraulic conductivity of the saturated and unsaturated zones, the negative percentage-clay term, and the permeability of the soil represent the apparent importance of media permeability both near the surface and at depth. The negative hydraulic-gradient term suggests that areas with more gentle slopes and presumably slower ground-water flow tend to have less likelihood of advection and dispersion of atrazine in the ground water. The number of registered irrigation wells within a 1.7-mile radius of the sampled well was the only land-use variable in these models and represented the effects of both irrigated agriculture and related chemical use in defining areas of ground-water contamination with nitrate and atrazine.

Model F used only three explanatory variables to account for about 61 percent of the variation in the concentration of atrazine in the ground water in study

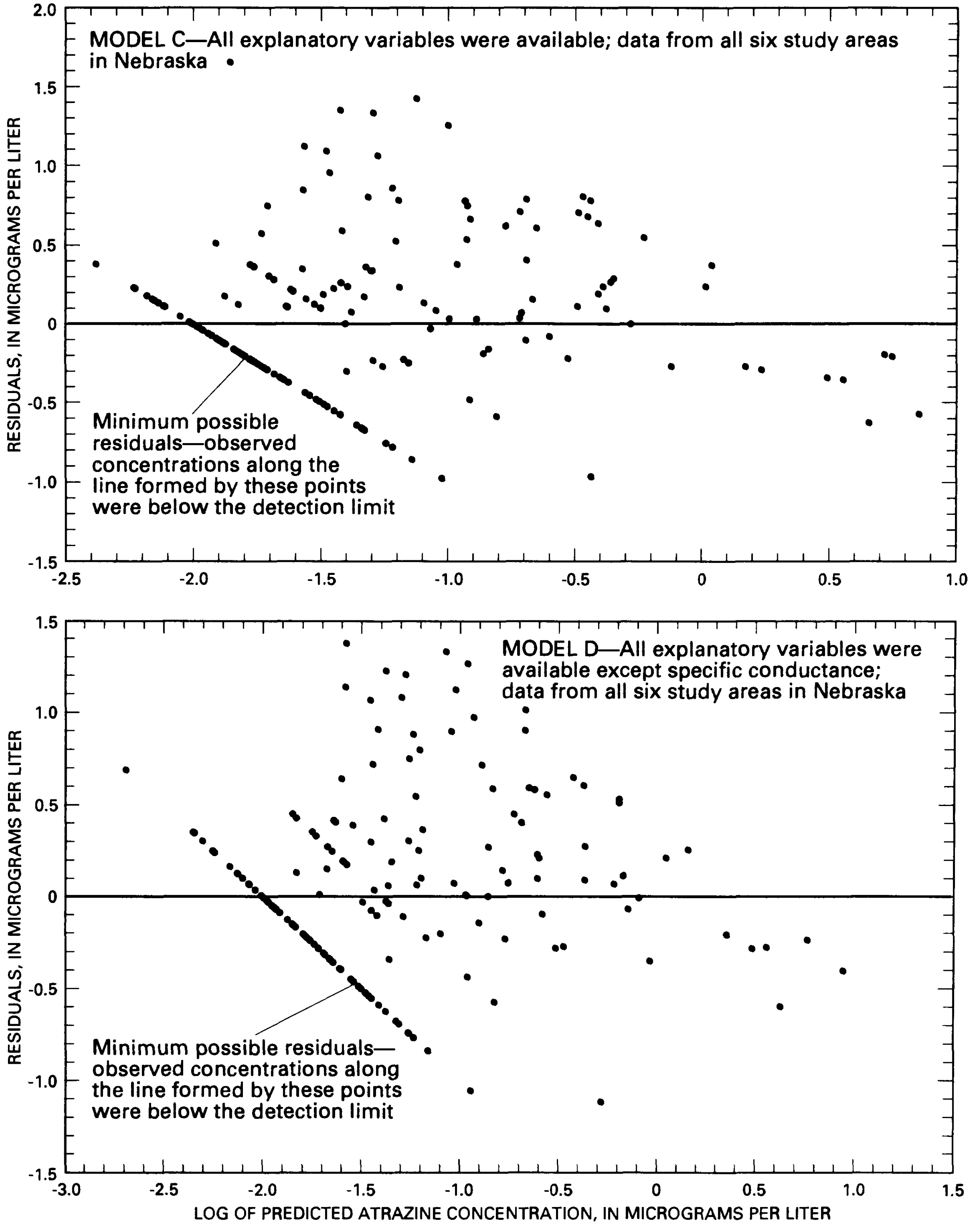


Figure 12. Residual plots for multiple linear regression models predicting atrazine concentrations in ground water.

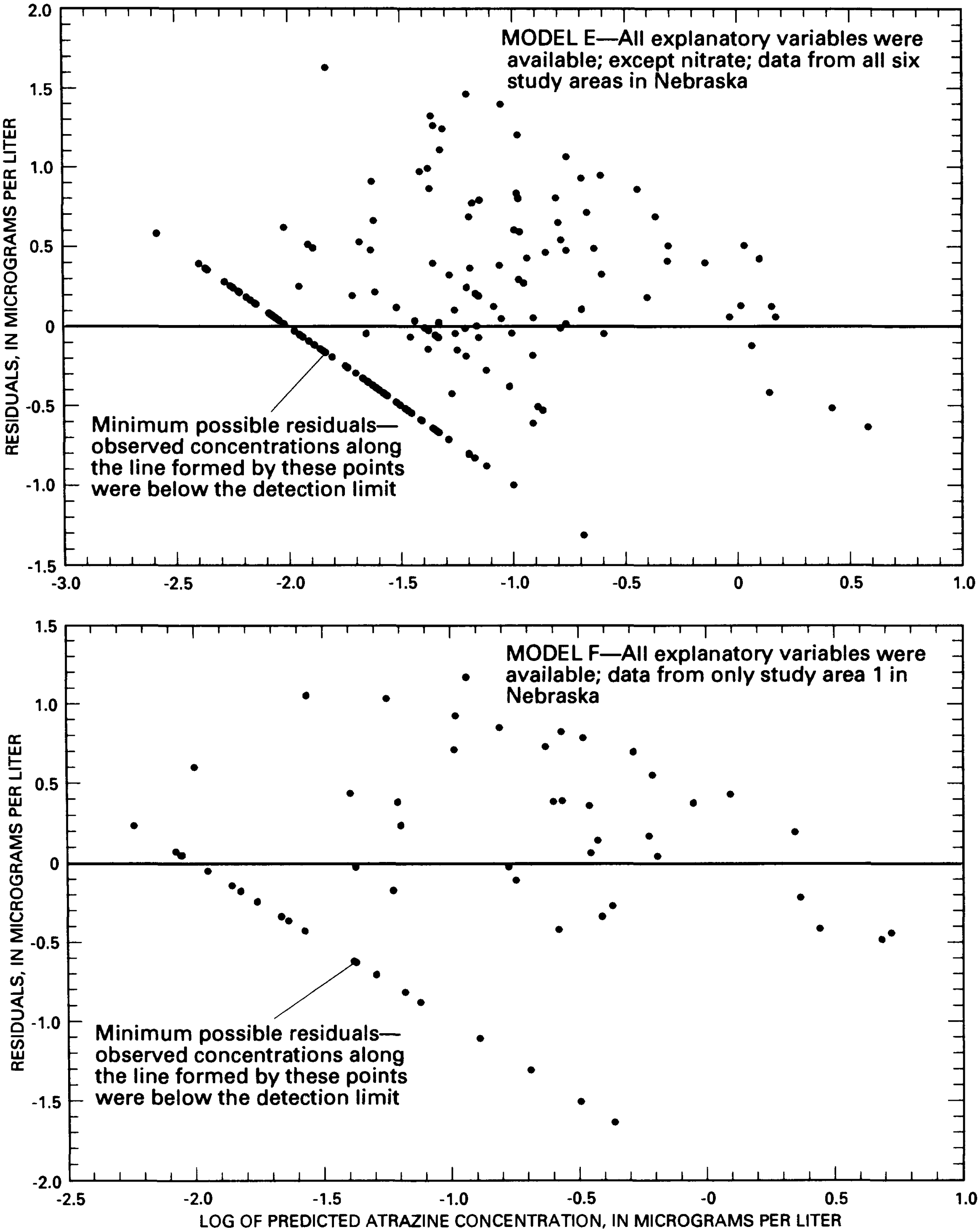


Figure 12. Residual plots for multiple linear regression models predicting atrazine concentrations in ground water—Continued.

area 1. The explanatory variables used were nitrate concentration, depth to water, and the number of irrigated acres within a 1.7-mile radius of the sampled well. The absence of soils explanatory variables in this model probably is the result of the relatively uniform distribution of silty to sandy-loam soils throughout much of study area 1.

Logistic Regression Models

A number of logistic regression models were produced using the presence or absence of detectable concentrations of atrazine in the ground water as the dependent variable. Three representative models are presented in table 6. One hundred and eighty two of the 210 wells from which ground-water samples were analyzed for atrazine were used to develop models G and H. Data from the remaining 28 wells contained missing values for some explanatory variables and were omitted from the analysis. Model I was produced with data only from study area 1 and used only 57 well samples. All three models correctly identified the presence or absence of atrazine in the ground water about 80 percent of the time. Water samples from wells that contained qualifiable atrazine concentrations, which were predicted to have a more than 50-percent probability of atrazine detection, were considered to be correctly identified by the models. Similarly, water samples from wells containing no qualifiable atrazine concentrations, which were predicted to have a 50-percent or lower probability of atrazine detection, were considered to be correctly identified by the models.

Models G and H differ from each other in the exclusion of nitrate concentration and specific conductance, respectively, as variables in the models. Model G suggests that atrazine detections in the High Plains aquifer are more likely in the study areas with larger specific-conductance values, slight hydraulic gradients, relatively permeable sediment in the unsaturated zone, shallow water tables, and soils with small clay content. The equation for model H shows similar relations with the hydraulic gradient and the average percentage of clay in a 60-inch soil profile. The equation for model H also suggests that areas with relatively large nitrate concentrations in ground water and relatively shallow wells have a greater probability of ground-water contamination with atrazine.

Model I was generated with data only from study area 1. Again, this restriction was used because the median atrazine concentration in water samples from study area 1 was larger than the median concentrations in each of the remaining five study areas at the 95-percent confidence limit as determined by the Kruskal-Wallis and Mann-Whitney tests. Model I used two explanatory variables, the average percentage of clay in a 60-inch soil profile and the number of registered irrigation wells within a 1.7-mile radius of the sampled well, to correctly identify the presence or absence of atrazine about 82 percent of the time. This model was the only one of the three logistic regression models shown that used a land-use explanatory variable.

Model Confirmation

Two separate approaches were used to confirm the validity of the models presented in tables 4 through 6. The first method involved the selection of eight registered irrigation wells in Merrick County (fig. 1), which is located immediately northeast of study area 1 and also borders the north side of the Platte River. Water samples were collected from each well in August of 1988 and were analyzed for nitrate and for atrazine. Ancillary data describing the appropriate explanatory variables also were collected. Estimates of the concentrations of nitrate and atrazine and the probability of detection of atrazine at or above the 0.02-µg/L qualitative detection limit were made using the models presented in tables 4 through 6. The results of these estimates are compared to the observed values in table 7.

The water samples from the confirmational wells contained no atrazine concentrations below the laboratories' quantitative detection limit for that method. Therefore, the abilities of these models to predict the absence of quantifiable atrazine concentrations in ground water were not evaluated.

The Wilcoxon signed-rank test (Minitab, Inc., 1989), a nonparametric test equivalent to the paired T-test, was used to compare the observed nitrate concentrations with the predicted concentrations from each model. Results of the tests indicated that the population of predicted values was not significantly larger or smaller than the population of observed values at the 95-percent confidence level. The p-values, the

Table 6. Logistic regression models with the probability of atrazine detection as the dependent variable

Explanatory variable	Intercept value or regression coefficient	Chi-square value	Probability of exceeding Chi-square
Model G—All explanatory variables except nitrate were available for inclusion in the model; data from all six Nebraska study areas.			
Number of samples used: 182			
Percentage of correctly identified detections: 79.5			
Percentage of correctly identified nondetections: 80.8			
Percentage of total correct identifications: 80.2			
Intercept	-1.512	7.21	0.0073
Specific conductance, in microsiemens per centimeter at 25 degrees Celsius	.00192	8.20	.0042
Transmissivity of the unsaturated zone, in feet squared per day	.00019	6.27	.0123
Gradient of potentiometric surface, in feet per foot	-593	5.75	.0165
Depth to water, in feet	-.0223	18.7	.0001
Average percentage of clay in the 60-inch soil profile	-.0840	8.57	.0034
Model H—All explanatory variables except specific conductance were available for inclusion in the model; data from all six Nebraska study areas.			
Number of samples used: 182			
Percentage of correctly identified detections: 77.4			
Percentage of correctly identified nondetections: 83.7			
Percentage of total correct identifications: 80.8			
Intercept	5.65	6.6052	.0102
Nitrate concentration, in milligrams per liter	.182	14.3	.0002
Gradient of potentiometric surface, in feet per foot	-959	11.0	.0278
Log of well depth, in feet	-2.08	4.83	.0280
Average percentage of clay in the 60-inch soil profile	-.0559	4.84	.0278
Model I—All explanatory variables were available for inclusion in the model; data from Nebraska study area 1 only.			
Number of samples used: 57			
Percentage of correctly identified detections: 88.9			
Percentage of correctly identified nondetections: 70.6			
Percentage of total correct identifications: 81.8			
Intercept	.813	.581	.446
Average percentage of clay in 60-inch soil profile	-.167	9.04	.0026
Number of registered irrigation wells within a 1.7-mile radius of the sampled well	.0329	6.11	.0134

Table 7. Comparisons of observed nitrate and atrazine concentrations in water from irrigation wells in Merrick County, Nebraska, in 1988, with predicted concentrations and probabilities of detection from selected models

Observed nitrate concentration, in milligrams per liter	Predicted nitrate concentration, in milligrams per liter		Observed atrazine concentration, in micrograms per liter[1]	Predicted atrazine concentration, in micrograms per liter				Predicted probability of atrazine detection		
	Model A	Model B		Model C	Model D	Model E	Model F	Model G	Model H	Model I
28	17.8	4.1	0.60	0.17	3.03	0.85	0.26	0.49	1.00	0.93
21	15.9	4.4	.30	.09	.38	.17	.16	.28	.95	.75
16	24.2	17.9	.50	.07	.33	1.46	.06	.46	.85	.98
8.8	26.8	14.9	.60	.39	.53	.61	.14	.87	.97	.94
18	19.0	15.1	.60	.09	.24	.23	.12	.44	.90	.87
16	16.7	6.8	1.40	.23	.71	.13	.16	.81	.97	.94
21	14.2	11.7	.30	.05	.09	.07	.04	.76	.71	.96
4.3	11.2	7.2								
P-values from Wilcoxon rank sign test[2]	.58	.16	P-values from Wilcoxon rank sign test[2]	.02	.40	.62	.02	--[3]	--[3]	--[3]

[1]One of the eight pesticide samples was damaged and not analyzed.

[2]The p-value is probability of producing test statistics that are equal or more extreme than the computed statistics from the same data sets if the observed and predicted concentrations are the same. A p-value of 0.05 or less indicates that the observed and predicted concentrations are different at the 95-percent confidence level.

[3]--, not applicable.

probability of producing test statistics that are equal or more extreme than the computed statistics if the observed and estimated concentrations were actually from the same population, for models A and B were 0.58 and 0.16, respectively.

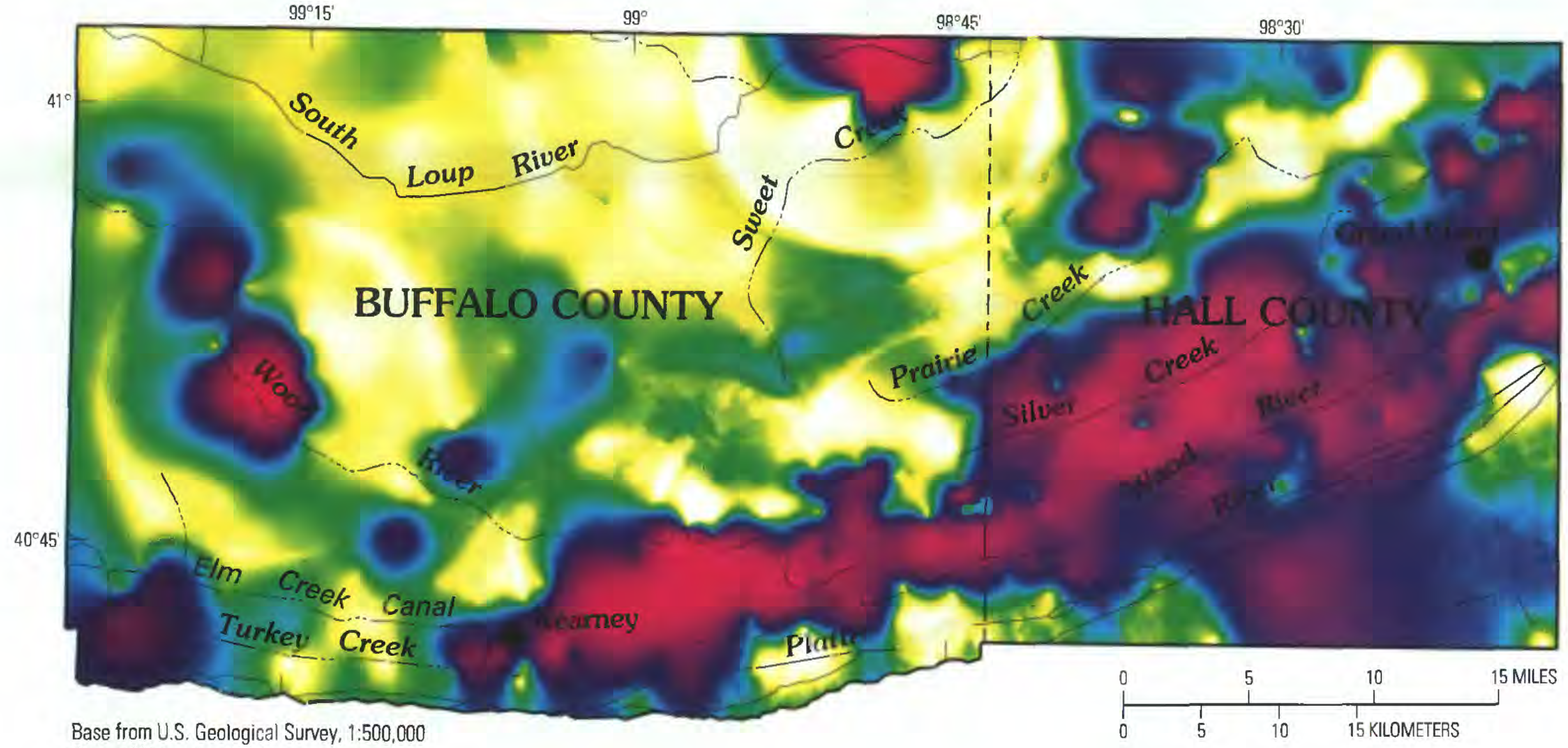
In contrast, the population of predicted atrazine concentrations produced by models C and F were significantly different (smaller) at the 95-percent confidence level from population of observed concentrations as determined by the Wilcoxon signed-rank test. The p-values produced by the tests for models C through F were 0.02, 0.40, 0.62, and 0.02, respectively. In comparing the logistic models for estimating probability of atrazine detections, model G predicted a probability of detection of 0.51 or more for only three of the seven observed detections. Models H and I correctly identified all seven sites with a probability of detection of 0.71 or more.

The second method of model confirmation was a subjective comparison of maps showing predicted concentrations of nitrate and atrazine and probability of atrazine detection in ground water in study area 1 with maps of observed ground-water concentrations prepared from water-quality data that were not used in developing the models. Figures 13 and 14 are maps showing observed concentrations of nitrate and atrazine, respectively, in ground water in study area 1. These concentrations were compiled by Exner and Spalding (1990), largely from the ground-water files of the Conservation and Survey Division of the University of Nebraska and the Nebraska Department of Health (Roy Spalding, University of Nebraska Water Center, written commun., 1991). Seven hundred and ninety three nitrate concentrations analyzed from 1984 through 1988 and 148 atrazine concentrations analyzed from 1979 through 1989 were used to generate figures 13 and 14.

The map of observed nitrate concentrations in ground water (fig. 13) was produced by kriging (as described by Oliver and Webster, 1990) the observed nitrate concentrations using an exponential function, a sample size of 84, and a raster cell size of 100 meters (table 8). A semivariogram showing the semivariance of z scores for observed nitrate concentrations between all pairs of points as a function of the distance between those pairs of points is in "Supplemental Information" section at the end of the report. The map of observed atrazine concentrations in ground water shown in figure 14 was contoured by hand rather than by kriging because the distribution of wells from which water samples were analyzed for atrazine was not uniform enough to yield semivariograms that were consistent with exponential, spherical, or linear mathematical functions that are used by the kriging method to describe the semivariance in most Earth-science applications (Oliver and Webster, 1990). The semivariograms also did not fit other mathematical functions available in the ARC/INFO raster-data analysis software.

Maps of study area 1 showing predicted ground-water contamination for each of the selected models were made by first interpolating a trend surface for each explanatory variable in the models by using the kriging, focal-sum, slope, grid, or inverse-distance weighting algorithms in the raster-data analysis software. Data describing the interpolation methods used for the explanatory variables are listed in table 8. Spatial-data sets used to create the trend surfaces had between 200 and 7,000 entries. A variety of kriged surfaces was created for five of the explanatory variables. The interpolation options for these explanatory variables whose semivariograms best fit the exponential, linear, spherical, or first-order polynomial mathematical functions (Environmental Systems Research Institute, Inc., 1992) were selected to represent the respective explanatory variable in the model(s). Semivariograms for each of the explanatory variables that were kriged, except for those kriged with the universal interpolation method and for which semivariogram analysis is not practical (Environmental Systems Research Institute, Inc., 1992), are shown as figures 18–22 in the "Supplemental Information" section at the end of the report. The surfaces for each model were then overlain, and the predictive equations were solved algebraically for each cell using the values of explanatory variables estimated in the trend surfaces. In cases where cell sizes varied among the explanatory-variable surfaces, the coarsest cell size was used. The maps predicting nitrate and atrazine concentrations and the probability of atrazine detections equal to or larger than 0.02 µg/L in ground water (figs. 15, 16, and 17) were compared to maps of study area 1 showing observed concentrations of nitrate and atrazine (figs. 13 and 14).

Although some differences exist between observed and predicted values in the distributions of nitrate and atrazine concentrations in study area 1, the overall similarities are readily apparent. The map of predicted nitrate concentrations generated by model B (fig. 15) shows a pattern of elevated nitrate

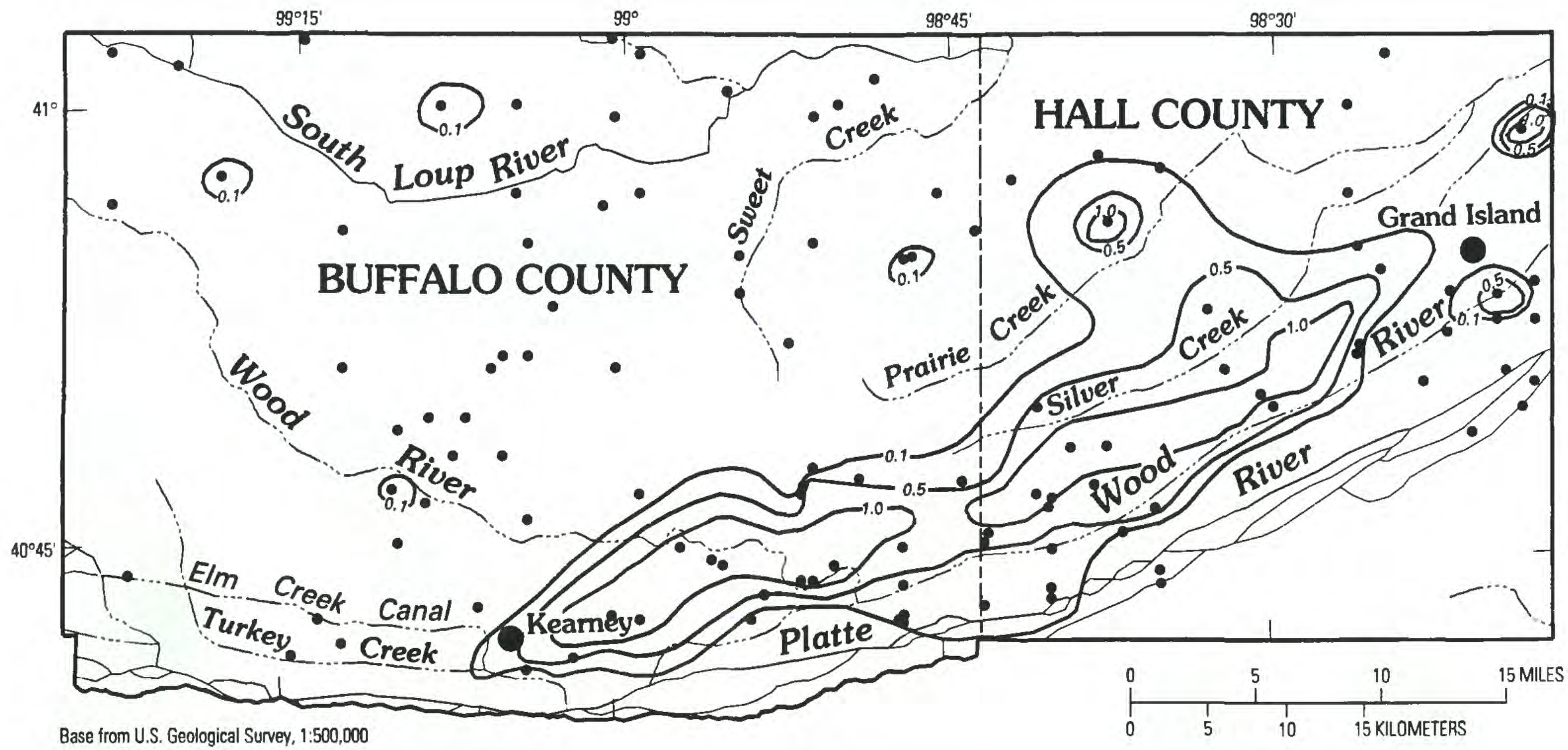


Base from U.S. Geological Survey, 1:500,000
State of Nebraska, 1984
Albers Equal-Area Conic projection
Standard parallels 29°30' and 45°30', central meridian 96°

EXPLANATION

Observed nitrate concentration, in milligrams per liter

Figure 13. Observed nitrate concentrations in ground water in study area 1 in Nebraska from 1984–88, using data compiled by Exner and Spalding (1990).



Base from U.S. Geological Survey, 1:500,000
State of Nebraska, 1984
Albers Equal-Area Conic projection
Standard parallels 29°30' and 45°30', central meridian 96°

EXPLANATION

—1.0— **Line of equal observed atrazine concentration in ground water—** Interval, in micrograms per liter, is variable

• **Well from which water was collected for atrazine analysis**

Figure 14. Observed atrazine concentrations in ground water in study area 1 in Nebraska using data compiled by Exner and Spalding (1990).

Table 8. Data describing the interpolation of observed nitrate concentrations and explanatory variables used in the construction of maps showing observed nitrate concentrations and predicted nitrate and atrazine contamination in ground water in study area 1 in Nebraska

Variable	Models using this variable	Interpolation method	Interpolation function	Cell size, in meters	Neighborhood function[1]	Sample size[2]	Radius, in meters
Observed nitrate concentration area 1[3]	NA[4]	Kriging	Exponential	100	NA	84	NA
Specific conductance	B	Kriging	Spherical	100	NA	24	NA
Average hydraulic conductivity of the unsaturated zone	B	Kriging	Spherical	100	NA	24	NA
Median completion date of irrigation wells within a 1-mile radius	B	Grid	None	100	NA	NA	NA
Nitrate concentration	F, H	Kriging	Exponential	210	NA	84	43,000
Depth to water	F	Kriging	Linear	180	Radius	NA	20,000
Number of irrigation wells in a 1.7-mile radius	F	Focal-sum[5]	NA	100	Circle	NA	2,740
Water level[6]	H	Kriging	Universal[7]	180	Radius	None	20,000
Water level[8]	H	Focal-mean	NA	180	Circle	NA	20,000
Gradient of the potentiometric surface	H	Slope	NA	NA	NA	NA	NA

Table 8. Data describing the interpolation of observed nitrate concentrations and explanatory variables used in the construction of maps showing observed nitrate concentrations and predicted nitrate and atrazine contamination in ground water in study area 1 in Nebraska—Continued

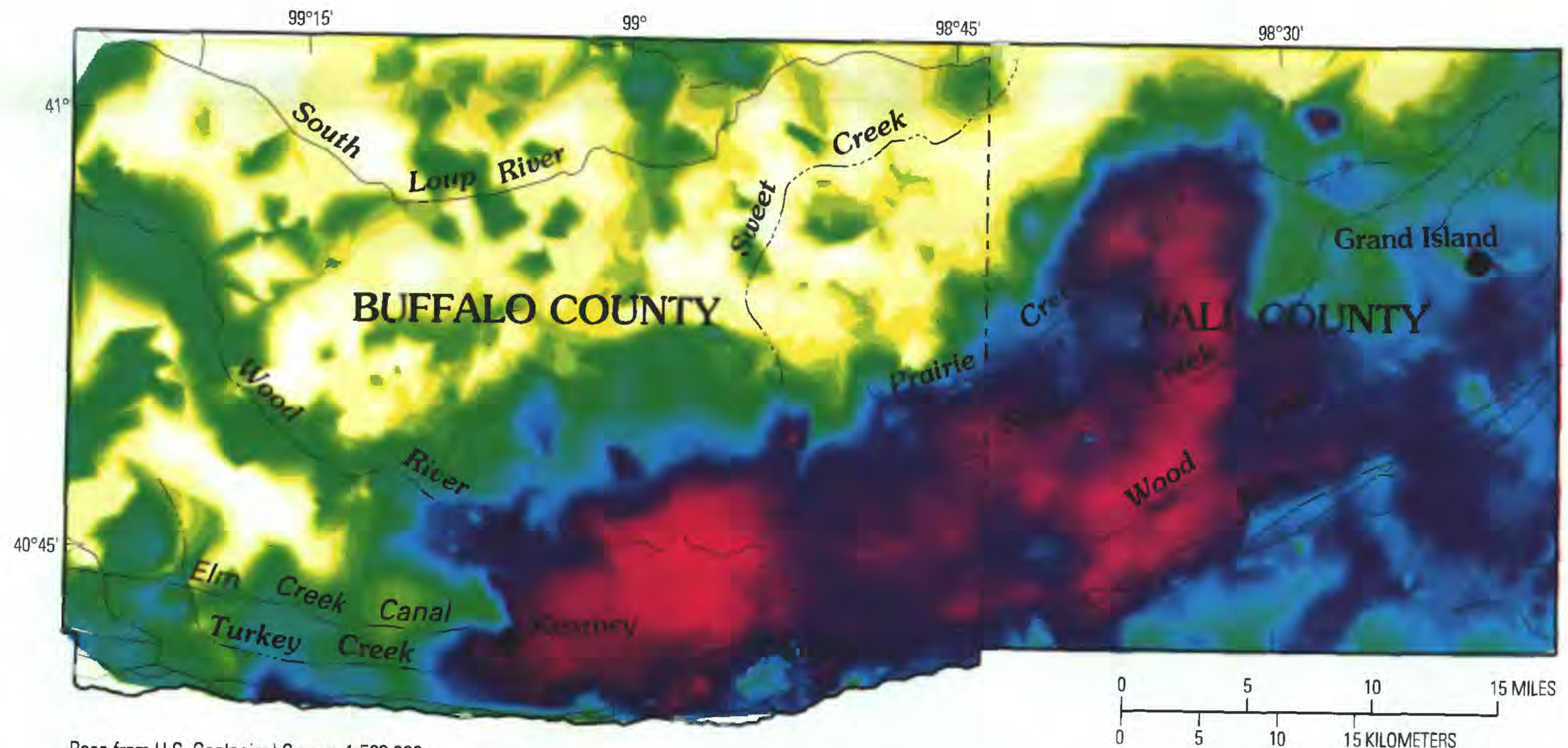
Variable	Models using this variable	Interpolation method	Interpolation function	Cell size, in meters	Neighborhood function[1]	Sample size[2]	Radius, in meters
Average percentage of clay in the 60-inch soil profile	H	Grid	None	45	NA	NA	NA
Log of well depth	H	Inverse-distance weighting	NA	100	NA	12	500

[1]Geometry of neighboring input cells considered in assigned interpolated values in the output cell.
[2]Number of neighboring input sample points for the interpolation of the value for each cell in the output grid.
[3]Roy Spalding, University of Nebraska Water Center, written commun., 1991.
[4]Not applicable.
[5]Output grid cells are assigned the sum of all cells within the specified group of input cells.
[6]This variable was used indirectly to produce the water-level variables for model H.
[7]A first-order polynomial function that approximates nonrandom change in spatial variables.
[8]This variable was used indirectly to produce the gradient of the potentiometric surface that was nsed in model H.

concentrations throughout the lowlands adjacent to the Platte River that is generally similar to the distribution of observed nitrate concentrations (fig. 13). The nitrate concentrations in the lowlands for the predicted and observed maps ranged from 10 to about 30 and 70 mg/L, respectively. Both maps also show several broader areas of nitrate concentrations in excess of 20 mg/L along the north side of the Platte River. The elevated predicted nitrate concentrations cover a broader area than the observed concentrations, and the areas of maximum predicted concentrations tend to be focused in a large area of south-central Buffalo County and in a series of smaller areas in western Hall County. The deviations of the predicted concentrations from the observed concentrations are believed to reflect the pattern of elevated specific-conductance values (not shown) in these areas, which include the effects of increases in other dissolved solids in addition to nitrate.

The distribution of observed and predicted atrazine concentrations using the regression and the logistic models are quite similar. Model F predicted atrazine concentrations in the lowland areas adjacent to the Platte River to range from 0.40 to 0.55 µg/L (fig. 16). The spatial distribution of the larger predicted concentrations agrees closely with observed values, although the observed values ranged from 0.10 to more than 1.0 µg/L in this area (fig. 14). North of the lowlands, model F predicted atrazine concentrations ranging from less than the 0.01-µg/L qualitative detection limit to about 0.25 µg/L. Observed atrazine concentrations for this same general area ranged from less than the 0.10 µg/L to about 0.10 µg/L, which indicates that the predicted values within this range are overestimated by the model (fig. 12). Several areas of relatively small predicted atrazine concentrations are located in the upland areas throughout most of Buffalo County and the northwestern edge of Hall County. These predicted areas of smaller atrazine concentrations are not evident on the map of observed concentrations, probably because these areas are used more for grazing and contain relatively few registered irrigation wells for sample collection. Just north of this area, predicted atrazine concentrations increase to about 0.25 µg/L again as the land surface drops into the South Loup River drainage system where the water table is shallower and irrigated agriculture is again more common.

The map showing the predicted probability of atrazine detections in the ground water using logistic regression model H (fig. 17) also compares favorably with the map of observed atrazine concentrations.



Base from U.S. Geological Survey, 1:500,000
State of Nebraska, 1984
Albers Equal-Area Conic projection
Standard parallels 29°30' and 45°30', central meridian 96°

EXPLANATION

Predicted nitrate concentration, in milligrams per liter

Figure 15. Predicted nitrate concentrations in ground water in study area 1 in Nebraska as determined by multiple linear regression model B, which used explanatory variable data from 1984–87.

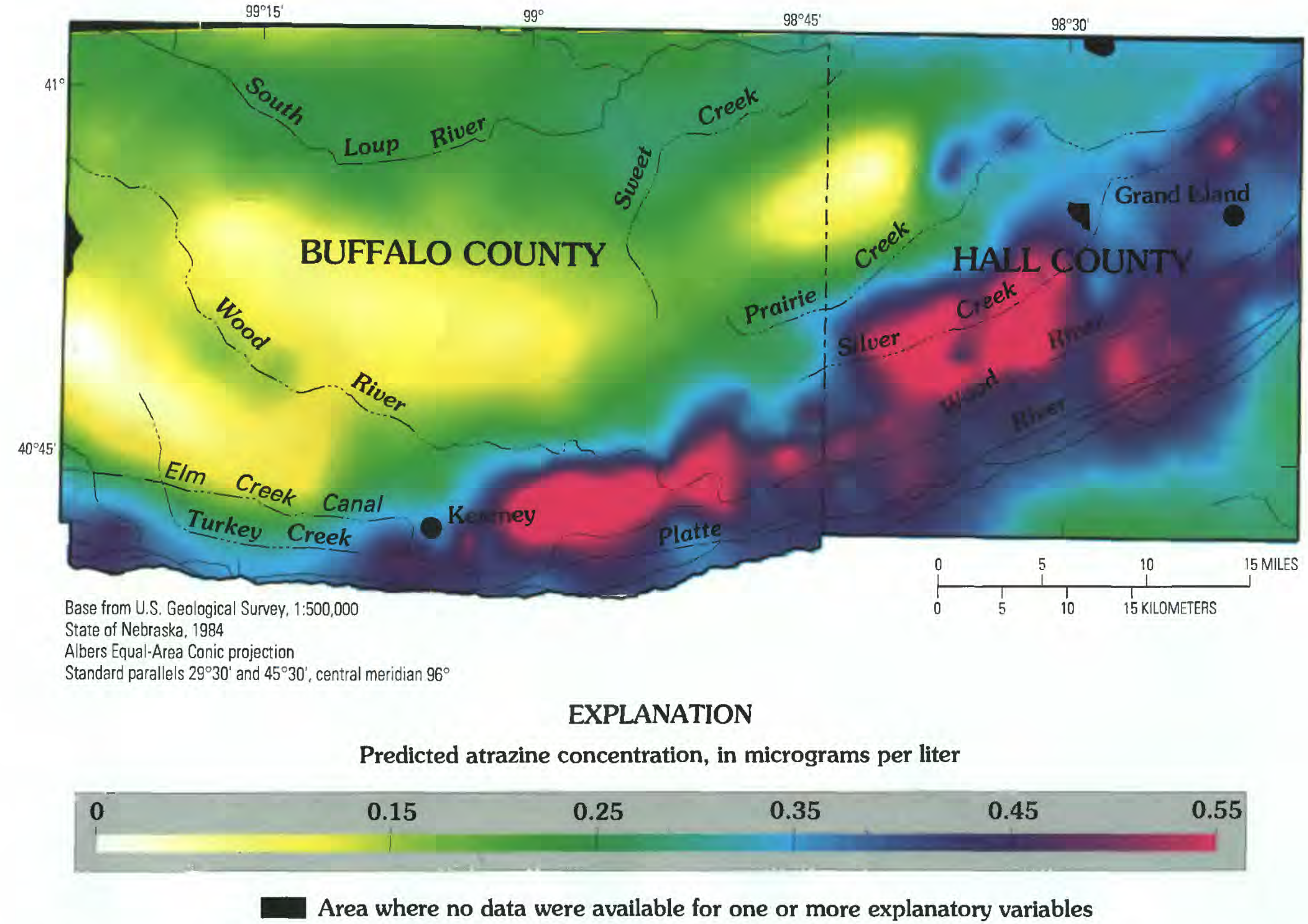


Figure 16. Predicted atrazine concentrations in ground water in study area 1 in Nebraska as determined by multiple linear regression model F, which used explanatory variable data from 1984–87.

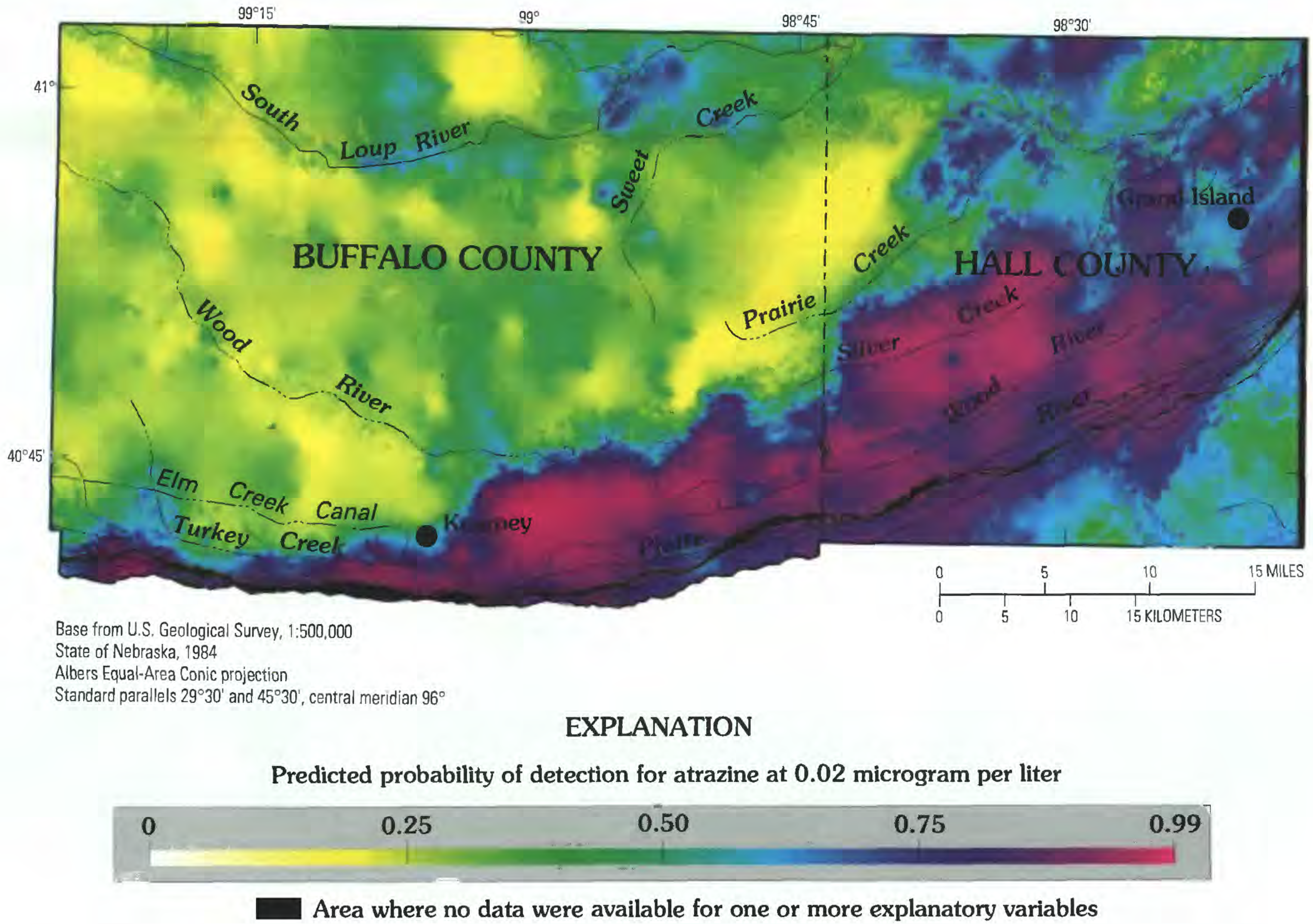


Figure 17. Predicted probability of atrazine detections of 0.02 microgram per liter or more in ground water in study area 1 in Nebraska as determined by logistic regression model H, which used explanatory variable data from 1984–87.

Figure 17 shows a 70- to 99-percent probability of atrazine detection equal to or greater than 0.02 µg/L in ground water in the lowland areas adjacent to the Platte River. This area of large detection probability extends just south of the Platte River in contrast to the map showing the observed atrazine concentrations. The difference may be due to the general lack of observed ground-water-quality data south of the river. Given the similarity of conditions on both sides of the river, it is likely that some atrazine contamination also may be present on the south side of the river. Figure 17 shows only a few areas where the predicted probability of atrazine detection in the ground water is between 0 and 15 percent. These areas generally coincide with upland areas with steep slopes where little irrigated agriculture occurs.

DISCUSSION OF MODEL RESULTS AND APPLICATIONS

The results of this study suggest that multiple regression techniques coupled with geographic information systems can be an effective means of identifying areas of potential ground-water contamination with nitrate and atrazine. Predictive equations can be produced using combinations of hydrochemical, hydrologic, soils, and land-use data that are available in a given area. The regression-model development process sorts out those explanatory variables that contribute significantly to the model and discards the others. Some understanding of basic hydrologic and contaminant transport is essential both to select explanatory variables for the regression process and to disregard those models that appear to violate basic hydrologic principles.

The principal importance of the models presented in this report lies not in their utility as predictive tools, but as explanatory tools to identify those quantified variables (and the underlying processes associated with them) that appear to have the most impact on nonpoint-source contamination of ground water by agricultural chemicals. Those processes appear to include the permeability of the soils and aquifer materials, the estimated rate of ground-water flow, the vertical proximity of ground water to the applied agricultural chemicals, and the areal extent, intensity, and duration of irrigated agriculture.

The models discussed here are not universal predictors of nitrate or atrazine but are unique to the selected areas for which they were developed. These models represent areas of relatively shallow, unconfined, aquifer systems underlying predominantly agricultural land. The explanatory variables used in these models and the relations they represent are functions of a unique blend of available data and the apparent dominant processes exerting the most effect on ground-water contamination in these areas.

Not all of the processes believed to affect nonpoint-source ground-water contamination by agricultural chemicals are represented in these models. Some explanatory variables, which intuitively would be expected to explain large portions of contamination variability, were not included because data for these variables were not readily available. An example is the absence in these models of a variable describing recharge from irrigation return flows. If data describing these explanatory variables were available, their inclusion in the models would be expected to increase the amount of explained variation (R-squared values) for the models.

It is clear from examining the confirmational tests and comparisons of the models that the nitrate models were not as effective in predicting areas of contamination as were the atrazine models. This is surprising because more nitrate data were used in generating the models than atrazine data, nitrate is applied at about 100 times the rate that atrazine is applied, nitrate is used on a greater variety of crops than atrazine, and nitrate does not tend to sorb onto sediment nor degrade in an oxidized environment as does atrazine. Perhaps the limited effectiveness in predicting areas of ground-water contaminated with nitrate is a result of the wide-spread use of nitrogen fertilizer in the study areas associated with the fact that the fate of nitrate in ground water is not fully understood. Also, because nitrate is used as an explanatory variable in many of the atrazine models, which explained more variation than did the nitrate models, it appears that as an explanatory variable nitrate concentration represents an apparent contaminant-leaching factor that was not available in another form in the nitrate models.

The methods presented here easily could lend themselves to the identification of a variety of nonpoint-source contaminants other than nitrate and atrazine in ground water. However, for the multiple regression methods to be successful, a range of contaminant concentrations must be present in the ground water. Otherwise, the potential for contamination of areas currently not contaminated could not be determined by this method. The logistic regression method is perhaps the more practical method when the target contaminants are pesticides because pesticides, when present, frequently occur at concentrations near the analytical detection limits. Also, the logistic regression method does not require a wide range of concentrations for the dependent variable.

In most cases it is necessary to acquire a considerable amount of water-quality and explanatory-variable data to predict areas of possible ground-water contamination with nitrate and atrazine. If one's sole purpose is to identify areas of current contamination, the most effective approach might be to simply collect and analyze water samples from that area. The methods described here are useful in determining the potential for ground-water contamination in an area with relatively uniform hydrologic and land-use characteristics for which some water-quality data are available.

Using the same techniques to predict nitrate and atrazine concentrations or probability of detections in another area or State where different kinds of data are available most likely would produce models that differ considerably from those presented here. However, many of the same basic concepts affecting the movement of water and contaminants through the unsaturated and saturated zones should be represented in models for both areas.

SUMMARY

Statistical techniques were used to relate nonpoint-source ground-water contamination by nitrate and atrazine to a variety of explanatory variables for six study areas in Nebraska. Water samples were collected from 268 wells in 12 counties from 1984 through 1987 and were analyzed for nitrate concentrations; water samples from 210 of the wells were analyzed for atrazine. A number of hydrochemical, climatic, hydrologic, soil, and land-use explanatory variables that could affect the contamination of ground water by agricultural chemicals were identified and quantified for each of the 268 wells.

Scatter and smoothed plots, simple correlation, multiple regression, and logistic regression methods were used to determine which explanatory variables were statistically related to ground-water concentrations of nitrate and atrazine. Regression models predicting nitrate and atrazine concentrations were produced that explained from 50 to 68 percent of the variation in the dependent variables. Explanatory variables used to predict nitrate concentrations represented the areal extent of irrigation development, which is an indirect measurement of the likelihood of a well intercepting contaminated ground water from other fields upgradient, drainage and permeability properties of the soil and aquifer materials, concentrations of other dissolved constituents in ground water, and the length of time irrigated agriculture has been employed. Explanatory variables used to predict atrazine concentrations represented a measure of other dissolved constituents in ground water, how close the water table lies to the land surface, drainage and permeability properties of overlying soils and aquifer materials, the slope of the potentiometric surface, which affects rates of contaminant advection and dispersion, the areal extent of irrigation development, and the temperature of the ground water.

Logistic regression models predicted the probability of atrazine concentrations larger than 0.02 μg/L. The explanatory variables used by these models represented concentrations of other dissolved constituents in the ground water, the slope of the potentiometric surface, drainage and permeability properties of overlying soils and aquifer materials, the distance contaminants must be transported through the unsaturated zone to reach the ground water, and the areal extent of irrigation development. These models correctly identified the presence or absence of detectable concentrations of atrazine about 80 percent of the time.

The accuracy of the models was checked by comparing predicted concentrations or probability of detections produced by the models with observed nitrate and atrazine concentrations in water samples from eight registered irrigation wells in Merrick County. Additionally, maps of predicted concentrations and probability of detections were produced for study area 1 and compared to maps of study area 1 produced from observed nitrate and atrazine concentration data not used in the development of the models. Although there were some differences between predicted and observed concentrations of nitrate and atrazine, the areal distributions of contaminated areas were generally in agreement.

The results of this study suggest that multiple regression techniques coupled with geographic information systems can be an effective means of identifying areas of potential ground-water contamination by nitrate and atrazine. The models produced by these methods are not universal predictors of agricultural-chemical contamination but are functions of the appa-

rent dominant processes in the study areas and the data that were available to quantify them.

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SUPPLEMENTAL INFORMATION

The semivariogram is a graphical display of the variance in z scores (the y axis) between all pairs of sample points separated by varying distances (x axis) and is considered a qualitative measure of the fit of the kriged data to one of several curves predicting variance with spatial change. The z score is a unitless standardization of the variable and is calculated by taking the difference between the value and the mean for the population and dividing by the standard deviation of the population. The semivariance of the z scores is one-half the average squared difference in z scores between pairs of input sample points separated by a given distance. Each kriging effort uses a mathematical function to approximate the spatial variation in z scores within the input sample points. The mathematical functions used for kriged variables in this report are exponential, spherical, or linear. By varying the sample size or radius used in the kriging process the fit of the kriged data may approximate selected predicted curves (figs. 18–22).

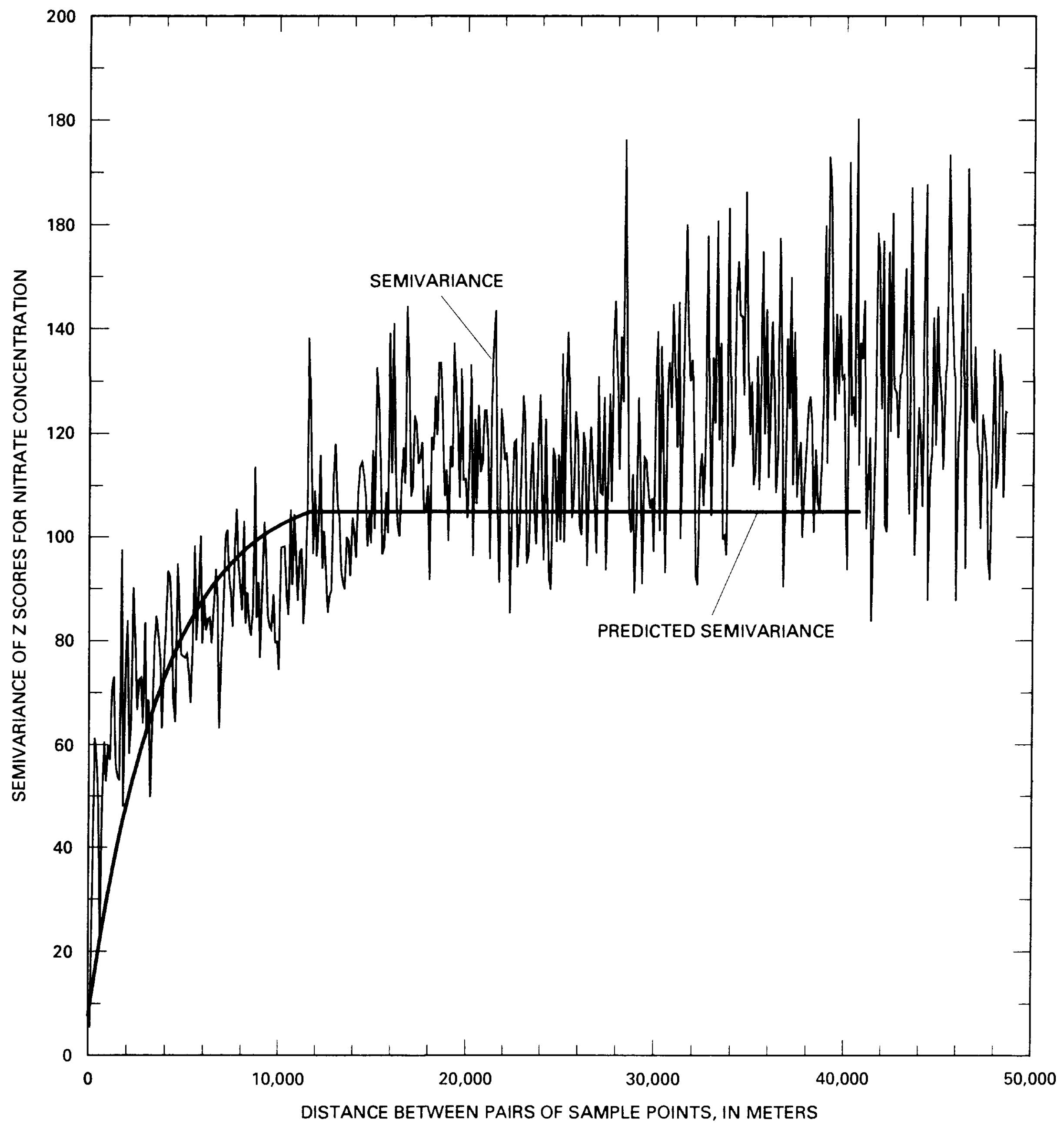

Figure 18. Semivariogram of kriged observed nitrate concentrations in ground water in study area 1 in Nebraska, 1984–88, using data compiled by Exner and Spalding (1990).

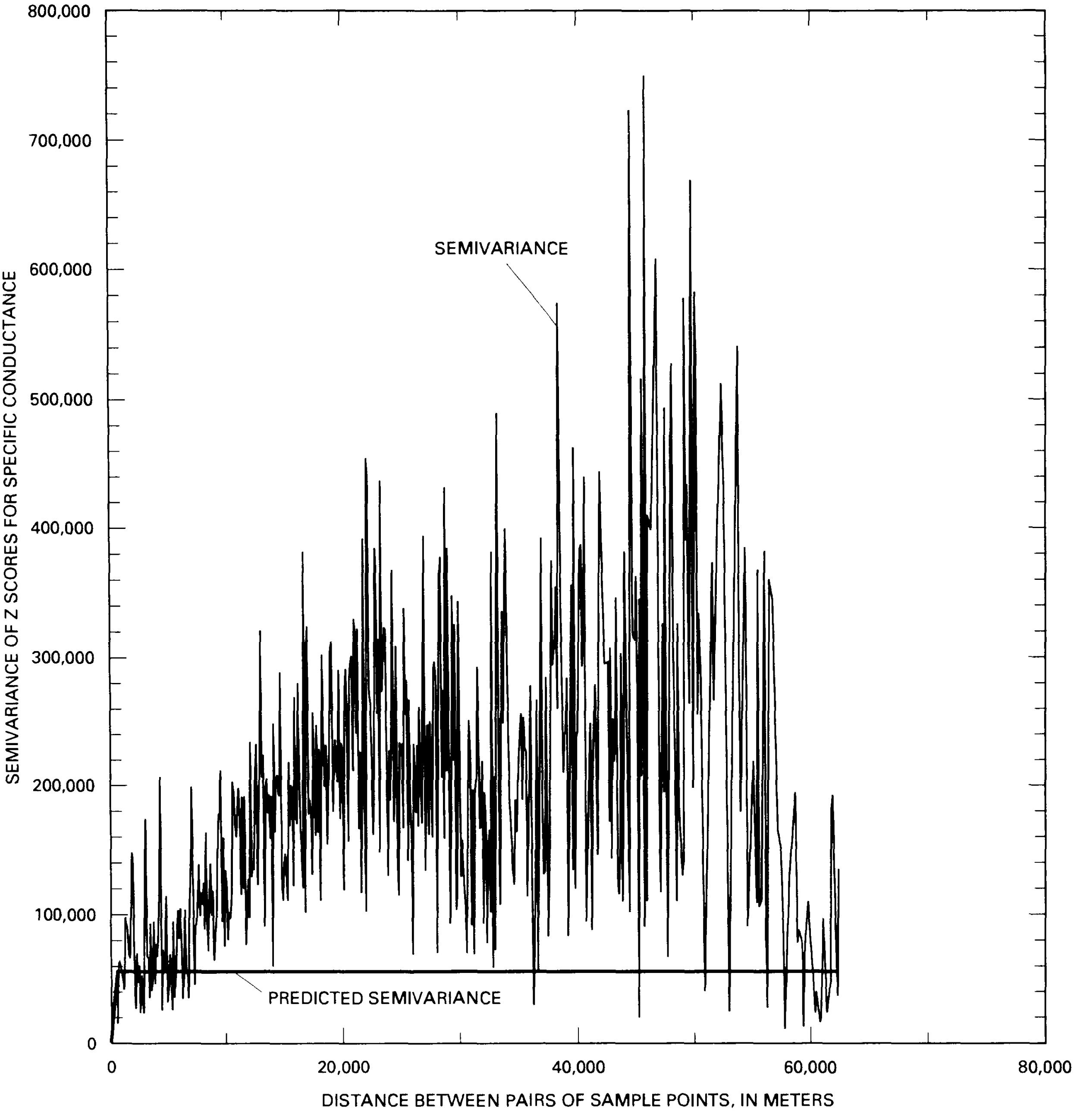

Figure 19. Semivariogram of kriged specific conductance for ground water in study area 1 in Nebraska, 1984–87.

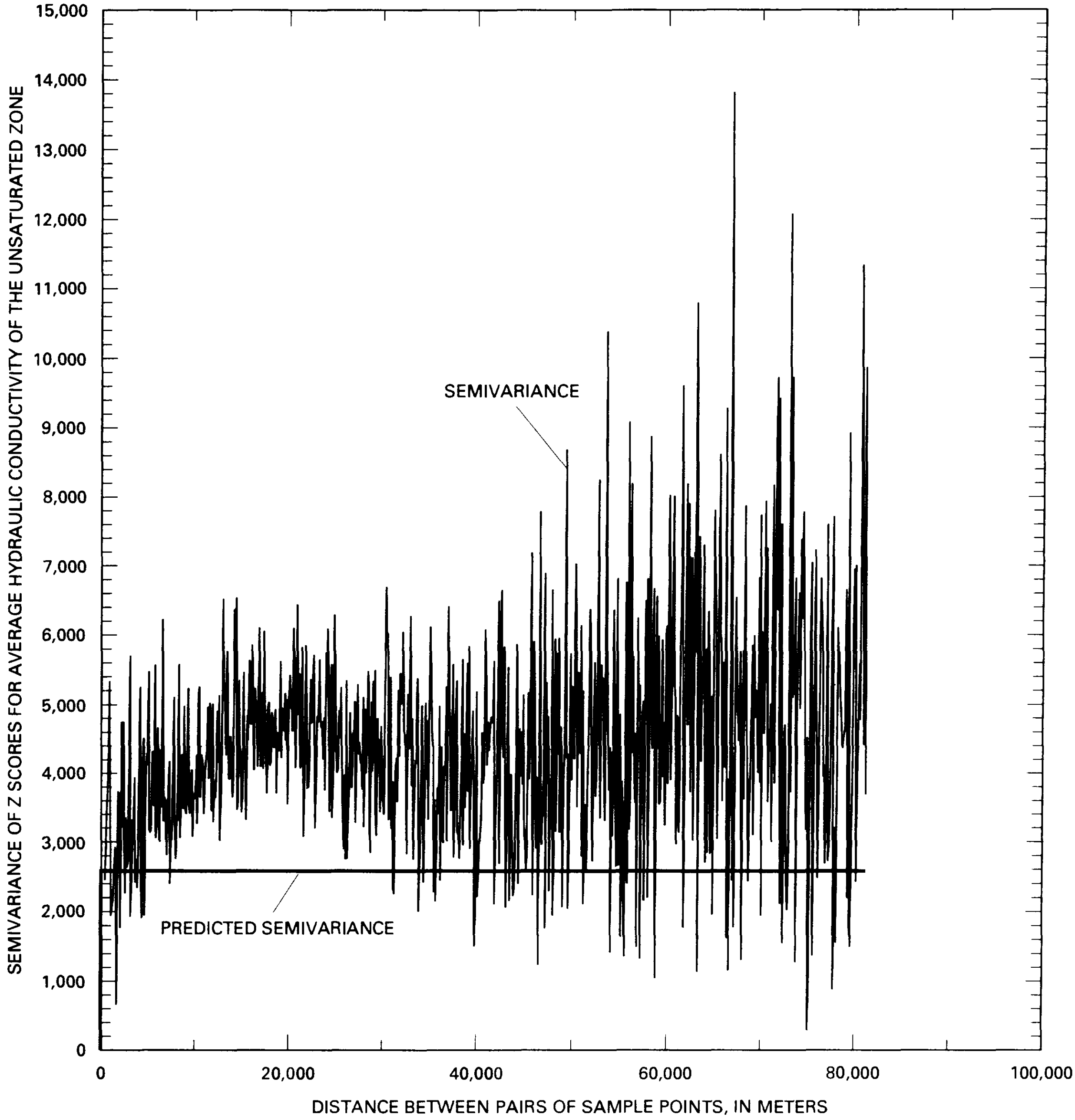

Figure 20. Semivariogram of kriged average hydraulic conductivity of the unsaturated zone in study area 1 in Nebraska, 1984–87.

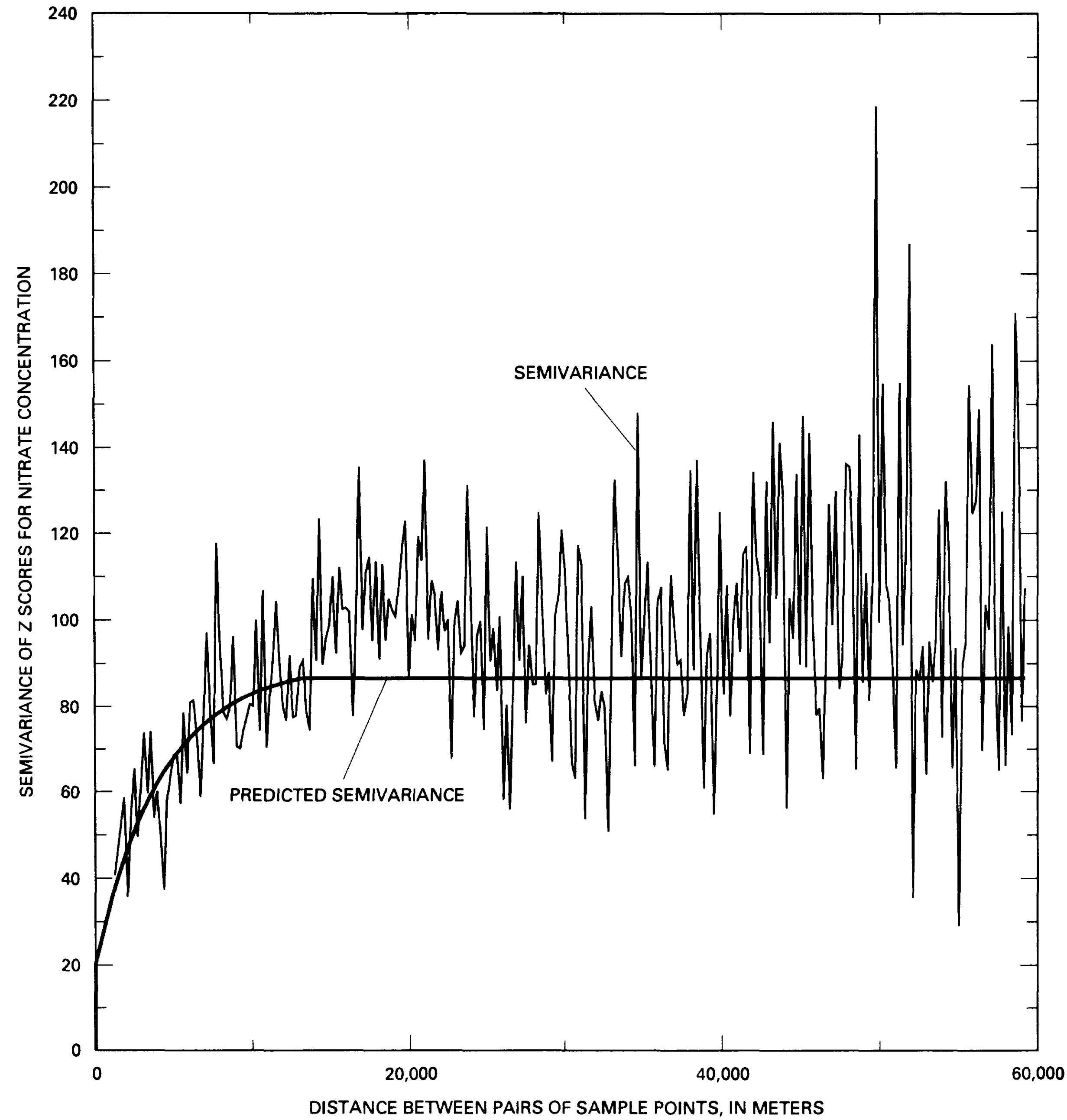

Figure 21. Semivariogram of kriged nitrate concentration in ground water in study area 1 in Nebraska, 1984–87.

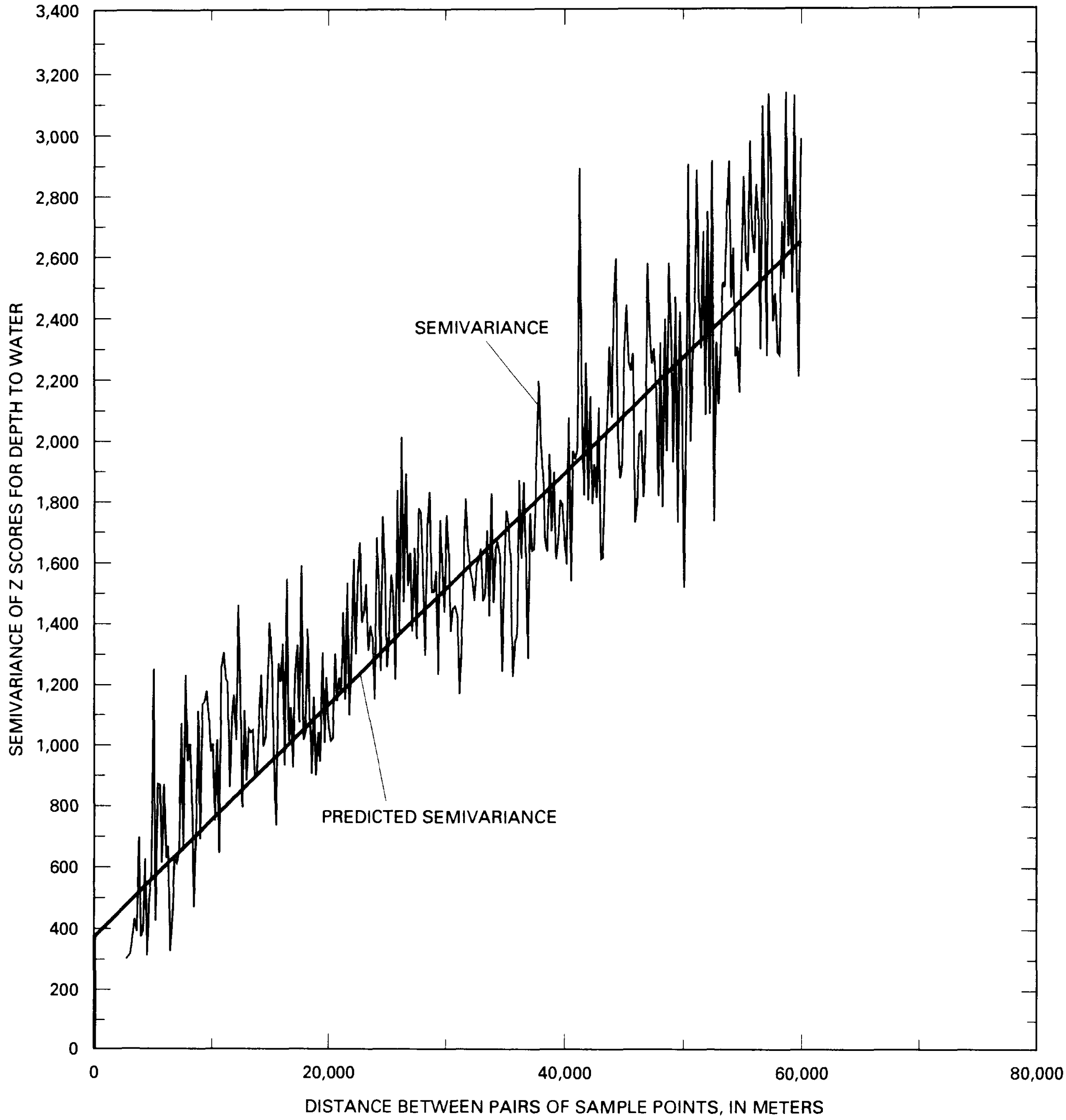

Figure 22. Semivariogram of kriged depth to water in study area 1 in Nebraska, 1984–87.

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