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GEOLOGICAL AND NATURAL HISTORY SURVEY
3817 Mineral Point Road
Madison, Wisconsin 53705

James Robertson, State Geologist and Director

HYDROGEOLOGIC AND LAND-USE CONTROLS ON ATRAZINE DETECTIONS IN DANE COUNTY, WISCONSIN

BY

M.A. Muldoon
M.F. Bohn
F.W. Madison
N.H. Richardson

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ABSTRACT

There is considerable interest in Wisconsin in relating soils, geologic, and hydrogeologic characteristics as well as land-use history to atrazine detections in order to improve the regulations and recommendations for the future uses of this pesticide and similar chemicals. At present, there are no clear-cut indicators to predict where atrazine detections may occur.

The goals of this study are to 1) inventory and automate land-use and natural resource information for Dane County, and 2) to identify the soils, geologic, and hydrogeologic features that make an area susceptible to atrazine contamination. Atrazine data for 397 wells in Dane County were compiled from the Grade A Dairy Farm Well Water Quality Survey, the Rural Well Survey, and Bradbury and McGrath's (1992) study.

Soils, geologic, and hydrogeologic data have been compiled in a variety of digital formats. The bedrock geology map for the county has been digitized. Digitized soils data have been used to rank soil map units on the basis of their ability to attenuate contaminants. A map of surficial geology has been developed using parent materials information contained within the Dane County Soil Survey. The locations of more than 2,900 wells in Dane County have been digitized. Data from the well constructor's reports (WCRs), including static water level, specific capacity information, and the driller's interpretation of the geology, have been entered into a relational database. A water-table map has been constructed using depth-to-water information from the WCRs and surface-water elevations. Data from the soil survey and from the WCR database have been used to update the depth-to-bedrock map for the county. Zones of contribution (ZOCs) have been determined for 397 sampled wells using GPTRAC, a particle-tracking model developed for the U.S. Environmental Protection Agency's wellhead protection program. Land-use data have been compiled from aerial photographs taken over 12 consecutive years (1979-1990), and atrazine usage has estimated on the basis of a given field's cropping history over that time interval.

A geographic information system was used to summarize and integrate the soils, geologic, hydrogeologic, and land-use data. Spatial exploration of the data, non-parametric cross-tabulations, and logistic regression were used to identify those variables of primary importance in predicting atrazine detections. Primary variables include 1) atrazine use, 2) presence of shale within the ZOC, 3) presence of Sinnipee dolomite as the uppermost bedrock unit over the ZOC, and 4) location in a discharge area. Secondary data trends were identified using logistic regression and cross-tabulation tests.

Logistic regression was used to incorporate both primary and secondary variables into predictive models. Models were developed for both atrazine detection and exceedence of PAL using all wells, wells in the glaciated area, and wells in the unglaciated area. The atrazine detection model developed using data from all wells had an overall predictive accuracy of 66% and was relatively unbiased with 69% of the detections accurately identified and 62% of the non-detections accurately identified. Stratification of the data and development of separate models for the glaciated and unglaciated portions of the county led

to improved overall predictive accuracy. Models to predict PAL exceedences tended to have good overall predicative accuracy but were highly biased and poor predictors of PAL exceedences.

ACKNOWLEDGMENTS

This project was jointly funded by DATCP and DNR through the Dane County Land Conservation Department (LCD). Information on field boundaries and cropping histories was provided by the Dane County LCD. Lee Gross of Dane County Extension helped estimate atrazine loading rates for various cropping histories. The PC ARC/INFO interfaces linking the land-use photos with the modeled ZOC boundaries were jointly developed by Dane County LCD and the University of Wisconsin Land Information and Computer Graphics Facility (UW-LICGF). Several individuals contributed greatly to this project; we thank the following people for their diligent efforts: Ken Bradbury, Dave Johnson, Jay Peterson, and Michelle Bridson, of WGNHS; Kevin Connors, Mike Oimoen, and Serena Slocum, of the Dane County LCD; Steve Ventura, of the UW-LICGF; Gary LeMasters, Lisa Morrison, Jeff Postle, and Jim Vandenbrook, of DATCP; and Mike Lemcke of DNR. We would also like to thank Andrea Belz who volunteered weeks of her time to help with the statistical analysis part of this project and Buzz Ostrom who assisted us in our understanding of Dane County bedrock stratigraphy and spent a day in the field showing us the various units.

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INTRODUCTION

Project Background

Atrazine, a popular and inexpensive herbicide, has been used extensively during the past 30 years in the corn-producing regions of the Upper Midwest. Atrazine provides effective control of broadleaf and grassy weeds; however, it has long been known that carry-over problems occur with continued use. Concern over the possible movement of atrazine to groundwater led the Wisconsin Department of Agriculture, Trade and Consumer Protection (DATCP) to monitor shallow wells installed downgradient of agricultural fields in the Lower Wisconsin River Valley (Postle, 1987). Sampling results indicated that atrazine was present in groundwater downgradient of irrigated agricultural fields with sandy soils and shallow water tables.

In 1988, DATCP conducted the Grade A Dairy Farm Well Water Quality Survey to determine the extent of pesticide contamination across the state. Five hundred and thirty four randomly chosen wells on Grade A Dairy farms were sampled for nitrate, atrazine, and three other pesticides. Twelve percent of the wells had levels of atrazine above the detection limit of .15 μg/l (LeMasters and Doyle, 1989). Wisconsin's groundwater standard for atrazine was initially 3.5 μg/l; since this is a health-based standard the preventative action limit (PAL) was 10% or .35 μg/l. In February 1992, a drinking water standard was defined and the groundwater standard was revised to include the concentrations of metabolites as well as parent atrazine. Both standards are currently 3 μg/l of atrazine and/or metabolites with a PAL of .3 μg/l.

In 1990, the Rural Well Survey was conducted by DATCP, the Wisconsin Department of Natural Resources (DNR), and Ciba-Geigy. Two thousand one hundred and eight-six samples sent in by homeowners were analyzed for triazine-based compounds (primarily atrazine and its metabolites) using an inexpensive immunoassay procedure (LeMasters, 1990). Statewide, approximately 16% percent of sampled wells contained detectable levels of triazines; in Dane County, an area of dairy-livestock agriculture with high corn production, triazines were detected in approximately 50% of the rural wells (LeMasters, 1990).

Concern over the presence of atrazine in rural drinking water supplies lead to the approval of the 1991 Atrazine Rule (chapter ATCP 30, Wis. Adm. Code) which established "atrazine management areas" where the use of atrazine is restricted and "prohibition areas" where the use of atrazine is prohibited.

In order to gain a better understanding of the extent and persistence of atrazine in groundwater, DATCP and DNR funded two site-specific studies in the glaciated and unglaciated areas of Dane County, Wisconsin. Chesters and others (1991), working in the glaciated portion of the county, concluded that the metabolite desethylated atrazine is as prevalent as parent atrazine in the shallow glacial-till aquifer near Waunakee, that groundwater containing atrazine may have recharged at least a decade ago, and that little atrazine and metabolite degradation is occurring in the saturated zone. They also concluded that while there is some evidence of point-source contamination at some of their sampled wells, most atrazine contamination is the result of normal field application of the pesticide.

Bradbury and McGrath (1992) examined the extent of atrazine contamination in bedrock aquifers in five small groundwater basins in western Dane County. The five-basin survey indicated that fractured-dolomite aquifers with thin soil cover may be more susceptible to atrazine contamination than aquifers with a thicker soil cover that have sandstone as the uppermost bedrock unit. A detailed groundwater inventory of the Fryes Feeder basin indicated that desethylated atrazine may be more persistent than parent atrazine, that the atrazine contamination in the basin has occurred within the last ten years, and that the unsaturated zone may be functioning as a continuing source of atrazine even after field-application of the pesticide has ceased.

These two site-specific studies provide detailed information on atrazine movement in specific hydrogeologic settings, however, there was also interest in trying to relate atrazine detections to land-use and hydrogeologic characteristics at a regional scale. Previous statewide investigations have had little success in correlating atrazine sampling results with patterns of soils or geologic materials (Kevin Kessler, verbal communication, 1990). Some areas that were assumed to be highly susceptible to pesticide contamination showed no atrazine detections; other areas that were assumed to be less susceptible to pesticide contamination did have detections. The investigation was limited in approach and these limitations probably led to the lack of correlation. Limitations include the following:

1. well locations were generalized;
2. geologic and hydrogeologic information used in the analyses was taken from state-wide maps and the data were not detailed enough to be used to adequately predict atrazine detections;
3. geologic and hydrogeologic information was examined at the location of the wellhead, rather than the area contributing water to the well; and
4. land use was not considered.

To better analyze the physical factors that might effect the distribution of atrazine detections, we decided to look at a smaller area, specifically Dane County, so that we could compile detailed geologic and hydrogeologic data, determine the land area most likely to contribute water to an individual well, and determine the land use in those contributing areas.

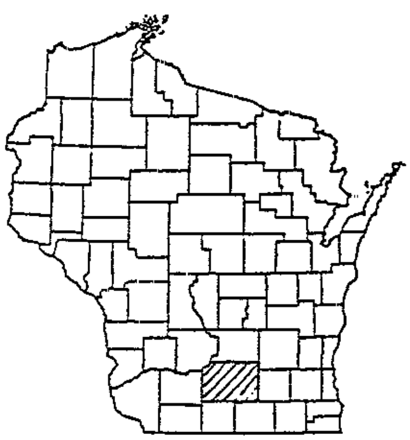
Purpose and Scope

The primary objective of this project is to determine the soils, geologic, and hydrogeologic factors that affect atrazine contamination of rural drinking-water supplies. Before we could begin to examine the physical controls on the distribution of atrazine detections, we had to determine the land area that contributes water to the sampled wells and then account for varying land-use practices within those areas. The project was conducted in four phases which are outlined below.

1. Development of GIS coverages of available soils, geologic, and hydrogeologic information.
2. Determination of the zones of contribution (ZOCs) of wells sampled for atrazine.
3. Estimation of atrazine application rates within the ZOCs.
4. Statistical analysis to examine the relationships among the hydrogeologic factors, land-use patterns, and the detections of atrazine.

Study Area

Dane County, located in south-central Wisconsin (Figure 1), was chosen as the study area for the following reasons: diversity of hydrogeologic settings; the large number of wells previously sampled for atrazine; primarily agricultural land use; and availability of some of the required resource data, specifically the bedrock geologic map and the soil survey, in digital format.



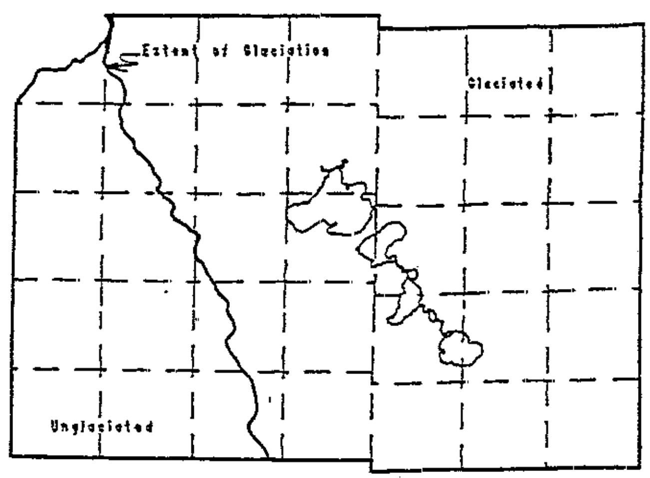


Figure 1. Map showing location of Dane County and extent of Pleistocene glaciation.

The bedrock geology of the area consists of a sequence of sandstones, dolomite, and shales of Cambrian and Ordovician age (Cline, 1965). The western third of the county was never glaciated (Figure 1) and the landscape consists of rolling, loess-covered bedrock hills dissected by a well-developed dendritic drainage pattern. These valleys are steep-walled with narrow valley bottoms that contain thick deposits of glaciofluvial sediment. The eastern two-thirds of the county is blanketed by up to 100 meters of unlithified sediment including tills, glaciofluvial, and lacustrine deposits. The drainage pattern is less well developed and the area contains many lakes and wetlands.

Residents of Dane County rely entirely on groundwater for their water supply. Most wells are developed in the Cambrian sandstones; however, unlithified sand and gravel deposits are sometimes used for water supply in the eastern two-thirds of the county and within the valley bottoms in the unglaciated areas. Unconfined or water-table conditions exist throughout the county and the sand and gravel aquifer appears to be in hydraulic connection with the deeper sandstone aquifer over most of the county (Rayne and others, 1993).

Dane County contains five distinct groundwater basins (Figure 2). These groundwater basins generally coincide with surface-water basins, however basin boundaries consist of groundwater divides as determined from Cline's potentiometric-surface map of the sandstone aquifer (1965). The Wisconsin River, Yahara River, and Sugar River are regional groundwater discharge areas. The discharge areas for the Pecatonica and Wolf-Fox basins lie outside Dane County.

Dairy farming is the predominant agricultural land use in the county; however, cash-grain farming, irrigated vegetable production, soybeans, fruit orchards, and tobacco are also important components of the county's agricultural economy.

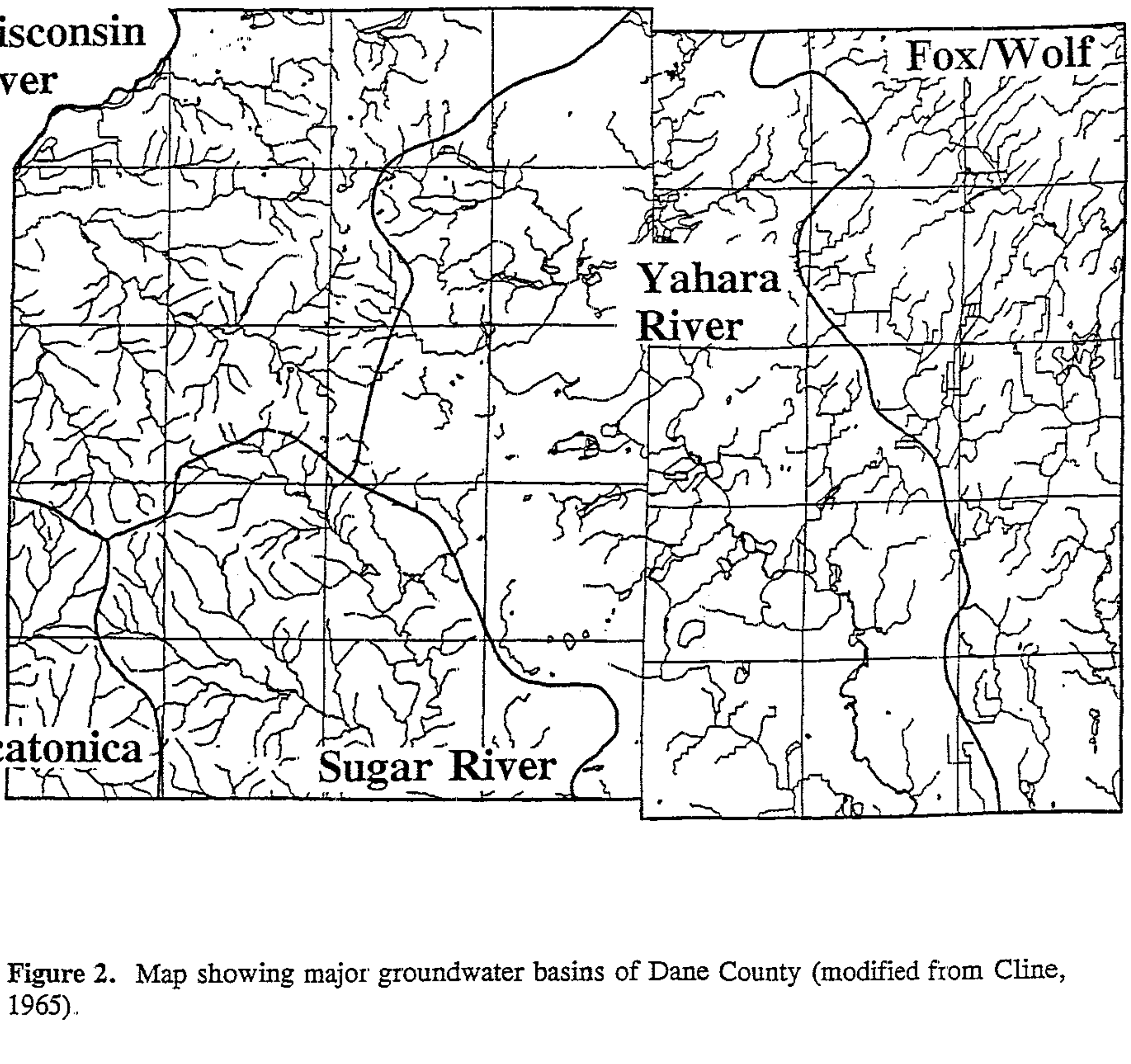


Figure 2. Map showing major groundwater basins of Dane County (modified from Cline, 1965).

Chapter II

GIS COMPILATION OF NATURAL RESOURCE DATA

Soils, geologic, and hydrogeologic data as well as cartographic data were compiled in a geographic information system (GIS) format using PC ARC/INFO software (Environmental Systems Research Institute, 1990). Base cartographic data include roads, surface-water features, township boundaries, and topographic map boundaries. Data that had been previously compiled include bedrock geology and soils. Additional data, including land use, well construction, atrazine concentrations, depth to bedrock, and elevation of the water table, were developed specifically for this project.

GISs are designed to store and manipulate spatial data; similar data are stored within a data layer called a coverage. ARC/INFO stores data as either points, lines, or polygons (areas). Each of these features can be assigned attributes (qualitative and quantitative) that describe the feature. In general, we used geo-relational database methods in which data tables were related through unique identifiers to geographic features in an ARC/INFO coverage. Our intent was to minimize the tabular data physically stored in the coverages, using instead the power of a relational data structure, and relying on dynamic joins to external data tables and lookup tables for analysis and display. One major advantage of this approach is an easier update procedure for attributes -- corrections can be made to one file instead of multiple files.

General Map Automation Approach

Data automated by WGNHS were located and plotted on full-size or reduced 7.5' United States Geological Survey (USGS) quadrangle bases, then digitized using the quadrangle map control in the state plane coordinate system. We used the PC ARC/INFO arc digitizing system (ADS) and ARCEDIT for digitizing and editing. The ARC/INFO Build and Clean commands, with a fuzzy tolerance of 5 meters or less, were used to identify errors and construct topological relationships for the features. Point features were assigned a unique identifier prior to digitizing. Linear features were generally digitized in stream mode. After check-plotting, editing, and archiving, line vertices were subsequently thinned using a line reduction algorithm (Douglas and Peucker, 1973) to reduce data volume while maintaining the character of the lines.

All data were projected to DaneTM, a local coordinate system developed for Dane County. This system uses local offsets to a transverse mercator projection similar to zone 16 of the Universal Transverse Mercator system. Units are meters and all coordinate values within the county are positive.

Large coverages were split into subareas, or tiles, based on geographic divisions. Some tiling schemes were based on the public land survey divisions; for example, soils were tiled by townships. In the case of the bedrock coverage, tiles were based on the USGS quadrangle map bounds.

Base Cartographic Data

Information from 1:100,000-scale USGS maps was used for cartographic presentation and reference. These data were originally developed by USGS, purchased from USGS in digital line graph format by WGNHS or other state agencies, and converted to ARC/INFO. Representations of the state trunk highways, county roads, and hydrography (surface waters) were obtained from the Wisconsin Department of Transportation. The LandNet representation of the public land survey was developed by WGNHS and DNR. Representation of 1:24,000-scale USGS quadrangle map boundaries and coordinate registration tics were mathematically generated by WGNHS.

Water-Quality Database

DATCP provided the database containing atrazine sampling results and well locations. Location information generally included owner's address and a township/range/section location specified to the ¼-¼ section. The 397 wells were sampled as part of the Grade A Dairy Farm Well Water Quality Survey (LeMasters and Doyle, 1989), the Rural Well Survey (LeMasters, 1990), or Bradbury and McGrath's (1992) study. The wells were identified through the Wisconsin Unique Well Number assigned to them as part of the various sampling programs. We determined more detailed well locations using a combination of methods, including aerial photographs, historical plat books, telephone directories, and field work. Well locations were then plotted onto 1:24,000-scale topographic maps and digitized.

Well Constructor's Report Database

Domestic well constructor's reports (WCRs) can provide the data necessary to construct water-table maps, calculate hydraulic conductivities, estimate porosities, and interpret bedrock geology. WCRs have been required for all domestic wells in Wisconsin since 1937. This provides an extensive and readily available source of subsurface data for most inhabited parts of the state. The reports include a legal description referencing the public land survey, an owner's name and address, information about well construction, results of a pumping test, and a description of the geologic materials encountered during drilling. Data reported are of varying quality. To use them effectively, we first selected the reports with the most complete information and then plotted selected wells on 1:24,000-scale topographic maps.

The locations of more than 2,900 of the approximately 13,500 wells in Dane County have been plotted on topographic maps and digitized into an ARC/INFO coverage. Data from the WCRs have been entered into a database along with indicators of locational accuracy and the land-surface elevation as determined from topographic maps. A unique identification number was assigned to each well and was used to relate the information in the WCR database to the well locations in the coverage.

Water-table Map

Some of the methods for determining the land area contributing water to a well, require an accurate water-table map. Cline's (1965) 1:100,000 scale map of the potentiometric surface in the sandstone aquifer is based on a limited number of data points. In addition, it was not clear that the potentiometric surface within the sandstone aquifer would coincide with the water table in all portions of the county. For these reasons, we developed a 1:100,000 scale water-table map based on the water levels reported for wells in the WCR database and surface-water elevations.

A computer-generated water-table map was created using the contouring package SURFER (Golden Software, 1990). Data used to generate the map included approximately 2,600 water-level elevations from the WCR database and over 2,000 digitized surface-water elevations. Computer contouring methods use various algorithms to estimate values at regularly-spaced grid nodes from irregularly-spaced data points. The configuration of the resulting map is somewhat dependent on grid size and choice of algorithm. For the water-table map of Dane County the minimum curvature algorithm was used with a grid size of approximately 800 m^2 (approximately 1/2 mi^2).

In order to check the accuracy of this contouring procedure, the resulting computer-contoured map was compared to 1:24,000 scale water-table maps of the Upper Black Earth Creek watershed (Muldoon, 1992). Visual inspection indicated that the contour lines were quite similar. The computer-contoured 1:100,000-scale water-table map was hand-edited and then digitized.

Soils Coverage

In the early 1980's, the Dane County soil survey was converted to a set of ARC/INFO coverages as part of the Dane County Land Records Project (Chrisman, 1986). WGNHS obtained these data from the Dane County Land Conservation Department (LCD). The individual soil map sheets had been digitized, transformed to DaneTM coordinates, and tiled along public land survey township boundaries. WGNHS performed some editing, attribute checking, coordinate transformation, and edge-matching of adjacent coverages. Tables of soil map unit attributes were obtained from the printed *Soil Survey of Dane County* (Glocker and Patzer, 1978) and from the SOIL5 database (U.S. Department of Agriculture Soil

Conservation Service, 1987). For this study, we developed attributes for the soil contaminant attenuation model ratings, soil parent materials, and soils with shallow bedrock. These coverages, derived from the digital soils data, are described below.

Soil Contaminant Attenuation Model -- SCAM2

The soil contaminant attenuation model (SCAM2) is a conceptual model that ranks soils on the basis of seven chemical and physical characteristics (Table 1) that affect the soils' ability to lower the concentration of potential pollutants applied at the land surface (Cates and Madison, 1990). Weighted values are assigned to each of the selected characteristics; those values are totaled for each soil map unit. The soil map units, based on those scores, are assigned to one of four classes (least, marginal, good, best) reflecting their contaminant attenuation potential. For this project, each soil map unit in the Soil Survey was ranked. A lookup table was developed to relate the soil map unit attenuation rankings to the digital soils coverages. Soil contaminant attenuation maps were created for the ZOC for each sampled well.

The ranking scheme of the SCAM2 model uses those soil characteristics which influence water movement into the surface soil (infiltration) and cause water to move slowly through the subsoil (percolation) thus maximizing the contact between soil water and soil particles. Attenuation is accomplished by a series of processes that depend on this contact between percolating water and soil particles. Thus, the model is designed to evaluate the ability of soils to attenuate surface-applied contaminants such as those contained in animal wastes or in agricultural chemicals.

Most soils in Dane County have formed in silt or silt loam textured materials which overlie unlithified materials originating either from glacial activity or from rock weathering. The features that differentiate these soils in terms of their ability to attenuate contaminants are the degree to which the soils have been eroded, the thickness of the surficial silts, and the characteristics of the materials underlying these surficial silts. Erosion may remove the topsoil, often exposing the subsoil at the land surface. The resultant changes in soil characteristics can significantly reduce the soils's ability to attenuate contaminants. In those instances where soils have formed over bedrock, erosion not only changes soil characteristics but also significantly reduces the thickness of soil materials through which potential contaminants move. This thinning of the soil mantle further reduces the attenuation potential of the soil, and, in areas where the bedrock permits rapid infiltration (such as fractured dolomite or clean sandstone), increases the possibility for the direct introduction of contaminants to the groundwater.

Soil Parent Materials

To examine the influence of soils on groundwater quality from a different perspective than the SCAM2 model, map units from the Dane County Soil Survey were aggregated on the basis of similar parent materials--those materials in which modern-day soils have formed.

Table 1. Ranking system for evaluating the attenuation potential of soils.

	Classes	Weighted values
Texture[1] of surface (A) horizon	l, sil, scl, si	9
	c, sic, cl, sicl, sc	8
	lvfs, vfsl, lfs, fsl	4
	s, sl, ls, organic materials, and all textural classes with coarse fragment class modifiers	1
Texture[1] of subsoil (B) horizon	c, sic, sc, si	10
	scl, l, sil, cl, sicl	7
	lvfs, vfsl, lfs, fsl	4
	s, ls, sl, organic materials, and all textural classes with coarse fragment class modifiers	1
Organic matter content[2]	Mollisols	8
	Alfisols	5
	Entisols; Inceptisols; Spodosols	3
	Histosols; Aquic suborder; and Lithic, Aquollic, and Aquic subgroups	1
pH-Surface (A) horizon	>6.6	6
	<6.6	4
Depth of soil solum[3] (A + B horizons)	>40 in.	10
	30-40 in.	8
	20-30 in.	3
	<20 in.	1
Permeability[4]-subsoil (B) horizon	very low	10
	moderate	8
	high	4
	very high	1
Soil drainage class	well drained	10
	well to moderately well drained	7
	moderately well drained	4
	somewhat poorly, poorly, and very poorly drained; excessively well drained	1

[1] Soil textural classes: l = loam, sil = silt loam, scl = sandy clay loam, si = silt, c = clay, sic = silty clay, cl = clay loam, sicl = silty clay loam, sc = sandy clay, lvfs = loamy very fine sand, vfsl = very fine sandy loam, lfs = loamy fine sand, fsl = fine sandy loam, s = sand, ls = loamy sand, sl = sandy loam.

[2] Based on the ordinal, subordinal, or subgroup levels of the soil classification system; soils are assigned a lower number if they are wet or less than 20 inches thick over bedrock; see county soil survey report.

[3] Assign next lower value if bedrock is within 30 to 40 inches of the soil surface; this takes into account erosion that may have decreased soil depth. See descriptions of soil map units in county soil survey report.

[4] Based on the particle-size class at the family level of the soil classification system, type, and grade of structure, and consistence; with strongly contrasting particle-size classes, the most permeable size class should be used. See soil profile descriptions and classification table in county soil survey report.

The maps resulting from this aggregation helped to identify patterns of materials in the landscape including the distribution of silt-sized materials.

Most soils in Dane County have formed in "two-storied" parent materials consisting of differing thicknesses of silty materials over some other type of geologic material, (*i.e.*, sedimentary rocks, materials deposited by glacial ice or by meltwater associated with that ice). Following the melting of the glaciers, materials which were predominantly silt-sized (0.5-.002 mm) were deposited by the wind across much of the landscape. Subsequently, these silt deposits (loess) were moved around the landscape by a variety of geomorphic processes to the point that in-place loess deposits probably are rare in Dane County.

Table 2 summarizes nine categories of parent materials for Dane County soils. These categories indicate the geologic material immediately below the zone of soil formation or the lower parent material for soils developed in "two-storied" materials. Each soil map unit was

Table 2. Soil parent materials of Dane County.

	Thickness of Silt or Silt Coverings (inches)				
Geologic/Soil Material	0	1-15	16-30	31-48	>48
Dolomite bedrock		X	X	X	
Sandstone bedrock	X		X		
Shale bedrock		X	X		
Till - generally ranging from sandy loam to loamy sand in texture		X	X	X	
Sand and gravel, primarily outwash	X	X	X	X	
Silts - alluvium					X
Silts - loess and colluvium					X
Fine sand and silt, primarily lacustrine deposits					X
Organic deposits - plant remains in varying stages of decomposition.	X				

characterized in terms of the parent material classes listed in Table 2. A lookup table was developed so that data in the digital soils coverage could be used to generate maps of parent materials and maps depicting the thickness and distribution of silt-sized materials on the landscape. From a water-quality standpoint, the distribution of these silt-sized materials on the landscape is important because of their capacity for contaminant attenuation. Their textural and structural characteristics maximize contact between percolating soil water and soil particles; in a general sense, therefore, the thicker the sequence of silts, the greater the potential for attenuation.

Bedrock Geology

Maps of bedrock geology show the distribution of geologic units with the unlithified materials stripped way. The bedrock geology map of Dane County is mainly the work of Olcott (1972), and was compiled on 1:24,000-scale bases. His interpretations were based on outcrop information and a sparse network of drill holes. Olcott's map was modified between 1986 and 1988 by Roger Peters with the assistance of M.E. Ostrom, both of the WGNHS. Their modifications were based on information from additional drill holes, WCRs, and some field work.

The modified bedrock map was digitized from the 1:24,000-scale base maps by WGNHS. ARC/INFO coverages were edge-matched and tiled into 9 sub-areas for the county. Figure 3 shows the portion of the bedrock coverage for the Verona township. The map key contains the complete stratigraphic column for Dane County; units are arranged in order of decreasing age from the bottom to the top of the key. Not all units are shown in Figure 3; the oldest unit shown on the map is the Tunnel City sandstone which occurs in the valley bottoms. Platteville dolomite, the youngest map unit, caps the ridgetops in this area.

Depth-to-Bedrock Coverage

Olcott (1973) also compiled a depth-to-bedrock map (1:62,500-scale) as part of his series of maps on the geology of Dane County. The map has a 50-ft contour interval, but it also shows areas where the depth to bedrock was 5 ft or less. The map was updated for this project using information from the digital soils coverage and the WCR database, and the updated map was digitized.

The SOIL5 database contains the range of depths at which bedrock was typically encountered for those soil map units with shallow bedrock. A lookup table was developed that uses the digital soils coverages to generate maps showing shallow bedrock. We generated a map showing areas where bedrock was less than 5 ft from the land surface and added this information to Olcott's map.

Well constructor's reports note the driller's interpretation of the geologic units encountered during drilling and this information was used to estimate a depth to bedrock. Drillers use a variety of terms to describe weathered rock and so it is not always clear at which depth the uppermost bedrock is encountered. For this study, "soft sandstone", "creviced limestone", and "limestone with boulders" were not interpreted as bedrock. Over 2,700 of the wells in the WCR database penetrate bedrock. Data from these wells were plotted at a scale of 1:62,500 and used to update Olcott's map.

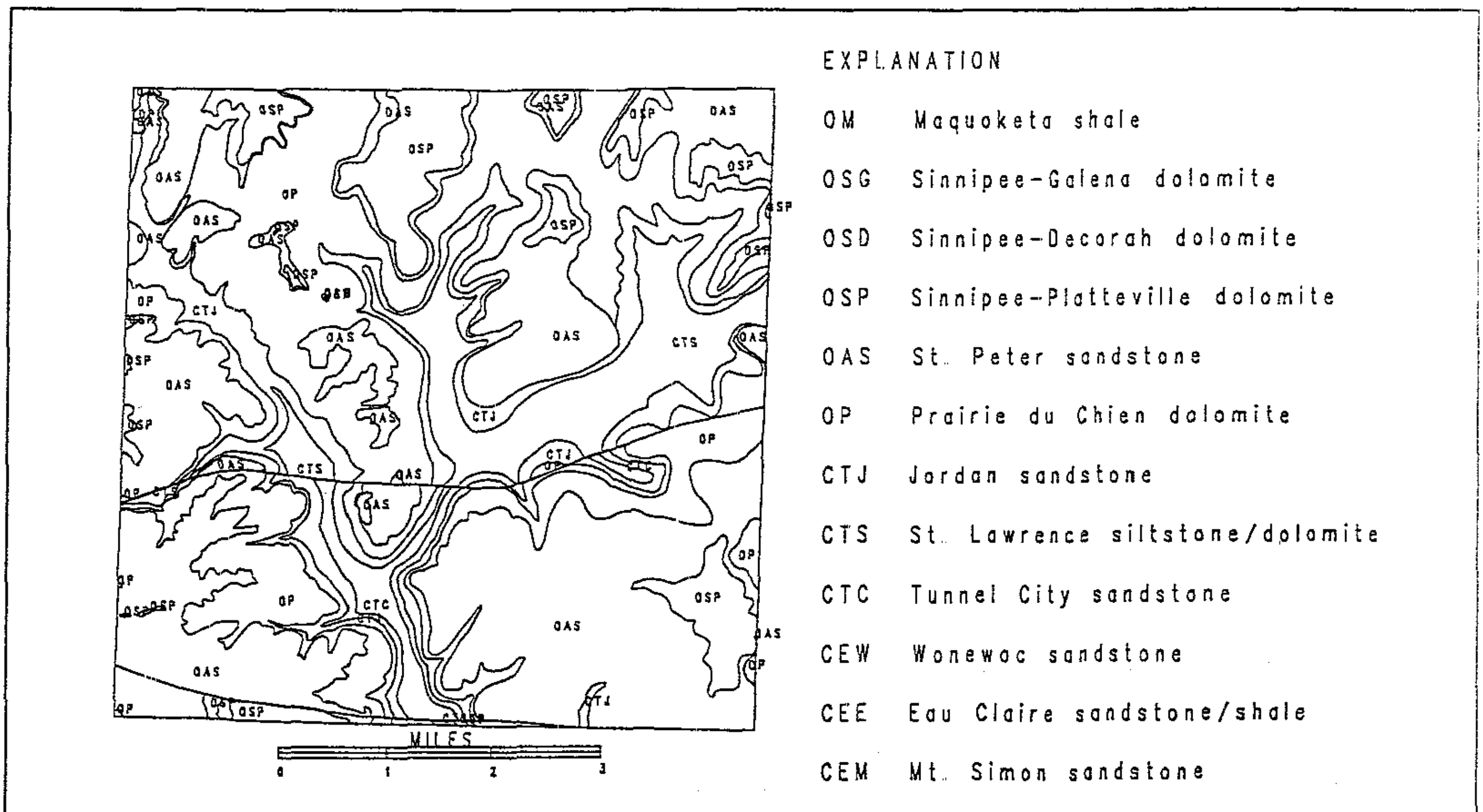


Figure 3. Portion of bedrock geology coverage, area shown is the Verona township.

Chapter III

ZONE OF CONTRIBUTION DELINEATION

Method Selection

Before we could begin to assess which soils, geologic, and hydrogeologic characteristics affected the distribution of atrazine detections, we had to determine the land-surface area around a well that was most likely to affect water-quality in that well. Previous studies that tried to relate water quality with land-use or hydrogeologic characteristics had used simple circles of a fixed radius (Barringer and others, 1990), or the physical characteristics of the 1/4, 1/4 section where the well was located (Kevin Kessler, verbal communication, 1990). While these techniques are simple to implement in a GIS environment, we did not feel that they were appropriate for shallow domestic wells completed in an unconfined or water-table aquifer. To choose a method, we evaluated several of the standard methods used to determine wellhead protection areas (U.S. EPA, 1987).

Some of the simpler methods of estimating the zone of influence (also called cone of depression or ZOI for the well) of a well are the calculated fixed-radius methods (U.S. EPA, 1987). These methods do not determine the entire land area contributing water to the well (also called the zone of contribution or ZOC for the well), rather, the assumption is made that the area within the well's cone of depression is the area most likely to contribute contaminants to the well. Figure 4 illustrates both the ZOI and ZOC of a well in an area with a sloping water table. This assumption is appropriate for wells with high pumping rates that are completed in confined aquifers or aquifers where the water table is relatively flat (Muldoon and Payton, 1993). Domestic wells tend to be pumped at low rates and do not develop a stable drawdown cone. For areas such as Dane County where the water table exhibits a great deal of relief, these methods tend to underestimate the land area contributing water to the well on the upgradient side and overestimate the contributing land area on the downgradient side. For these reasons we chose to evaluate the various flow-system mapping techniques.

The primary advantage of the various flow-system mapping techniques is that they estimate the ZOC of the well by taking into account the groundwater flow direction. Methods include 1) water-table mapping with manual determination of the ZOC (time-of-travel criterion can be calculated using Darcy's Law), 2) application of the Uniform Flow Equation (Todd, 1980) which calculates the horizontal width of the ZOC and the downgradient null point and is manually aligned with the flow direction, or 3) semi-analytical and numerical modeling methods. Given that we wanted to determine ZOCs for 397 wells, we chose not to use the manual mapping methods. The Uniform Flow Equation was developed for confined aquifers, however, it has been used for unconfined aquifers as well. The disadvantage of this method is that the width of the ZOC is very dependent on the hydraulic conductivity used in the calculation (Bradbury and others, 1991; Muldoon and

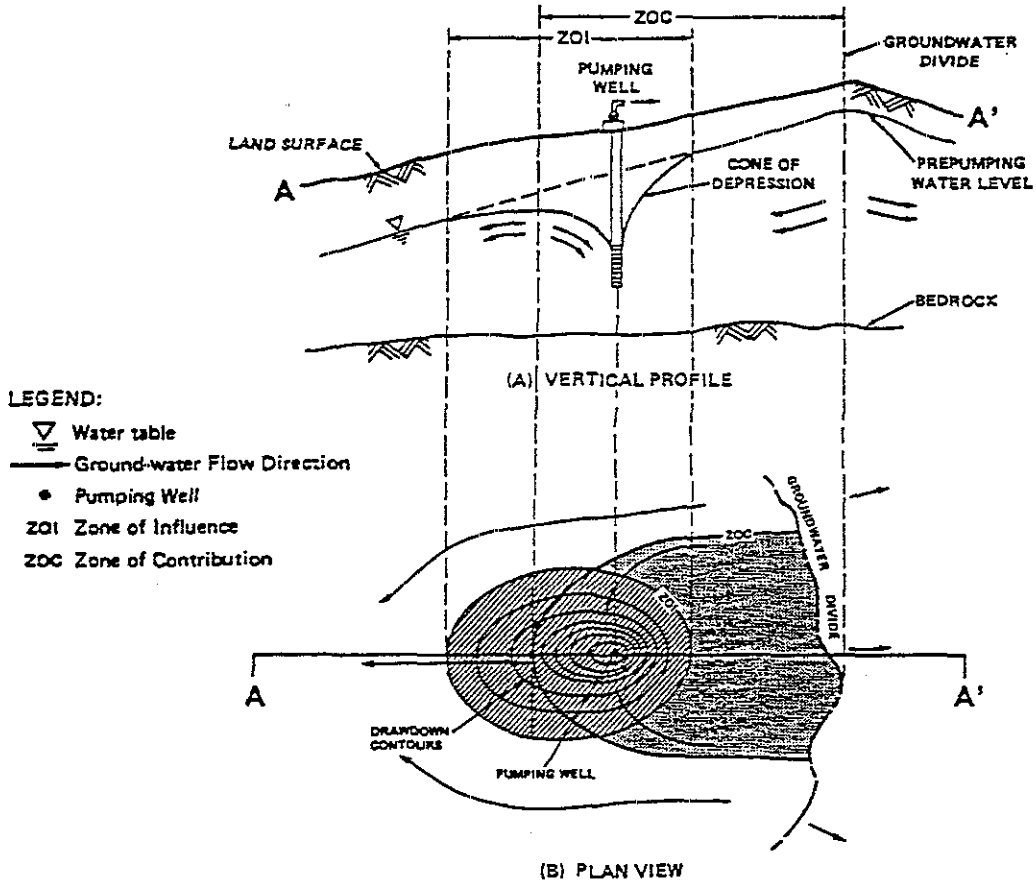


Figure 4. Diagram illustrating ZOI and ZOC for a well in an area with a sloping water table (Source: U.S. EPA, 1987).

Payton,1993). Due to these limitations we chose a modeling approach to calculate the ZOCs.

We chose to use the U.S. EPA's *WHPA* model (Blandford and Huyakorn, 1990) because 1) it is one of the more accurate methods of ZOC determination using the flow-system mapping technique, 2) it is widely available, and 3) its data requirements are realistic. *WHPA* is a public domain, two-dimensional, groundwater flow model that was developed by the U.S. EPA to assist with Wellhead Protection Area (WHPA) delineation. Several facts suggest that a three-dimensional modeling approach may be more appropriate for ZOC delineation in Dane County. The geology exhibits both spatial and vertical variability. The county contains several groundwater basins (see Figure 2, p. 5) and groundwater flow at basin boundaries is typically characterized by a significant vertical component. Developing the detailed hydrogeologic information required for such a three-dimensional groundwater flow model of the county was beyond the scope of this project.

The *WHPA* program contains three modules that can be used to calculate WHPAs; of these MWCAP and RESSQC depend greatly on the pumping rate of the well. These were not chosen, since domestic wells are usually pumped only intermittently and at low rates.

We chose to use the GPTRAC module which is a general particle-tracking model that can track particles through the groundwater flow system based solely on hydraulic head, independent of pumping rate. GPTRAC can be run in either a semi-analytical or numerical mode. The numerical option chosen requires hydraulic head values at the nodes of a regularly spaced grid. These head values can be the output of a numerical groundwater model or can be derived from a water-table map. Additional input requirements for GPTRAC include aquifer transmissivity, porosity, and aquifer thickness. ZOCs are then calculated for specified time periods. The model can incorporate horizontal anisotropy and heterogeneity if those data are available. Details on developing the model input and specific modeling procedures are described more fully in the following sections.

Hydraulic Head Grid

GPTRAC requires hydraulic head values for regularly-spaced grid nodes in order to track particles through the flow system. Data from the digitized, hand-edited, water-table map were exported from ARC/INFO into ASCII data files. For each topographic quadrangle, a file was created containing the contour-line head values and the surface-water elevations. These data were gridded using the minimum curvature gridding procedure of SURFER in order to create the hydraulic head input files needed for the GPTRAC model.

Aquifer Parameters

Aquifer parameters required for GPTRAC modeling include estimates of hydraulic conductivity, porosity, and aquifer thickness. An interactive PC ARCPLOT application, called PRETRAC, has been developed to assist hydrogeologists in developing input parameters for the particle-tracking model (Bohn and Muldoon, 1993; Muldoon and Bohn, 1993). PRETRAC spatially links the WCR database with water-table contours, bedrock geology, atrazine sample information, and cartographic reference databases. Table 3 lists menu options available in PRETRAC; these are explained in more detail in the following paragraphs.

To estimate aquifer parameters, one or more wells with constructor's reports are selected interactively (SEL_WCR) by drawing a circle centroid and radius. Information for selected wells is displayed through the use of a pop-up screen. Figure 5 shows the pop-up screen with information from a sample well constructor's report,

Hydraulic Conductivity and Aquifer Thickness

PRETRAC incorporates a FORTRAN version of the TGUESS program (Bradbury and Rothschild, 1985), which estimates hydraulic conductivity from specific capacity test data. For any given well, PRETRAC pulls information on well construction, pumping rate, and drawdown from a copy of the WCR database, writes an input file for TGUESS, estimates the

Table 3. PRETRAC interface options.

Menu options	Interface functions
SEL_WCR	Choose well constructor's reports to view
WCR_TGUESS	Run the TGUESS model for a well with constructor's report
TGUESS_2_WQ	Assign model results to a sampled well
EDITWQ	Edit the GPTRAC parameter file
WQ_WITH_T	Show which sampled wells have parameters assigned
SEL_4_GPT	Select wells for GPTRAC modeling
DUMPGPT	Dump the parameter files for the selected wells
MAKEWIN	Make a window to create the GPTRAC hydraulic head grid file

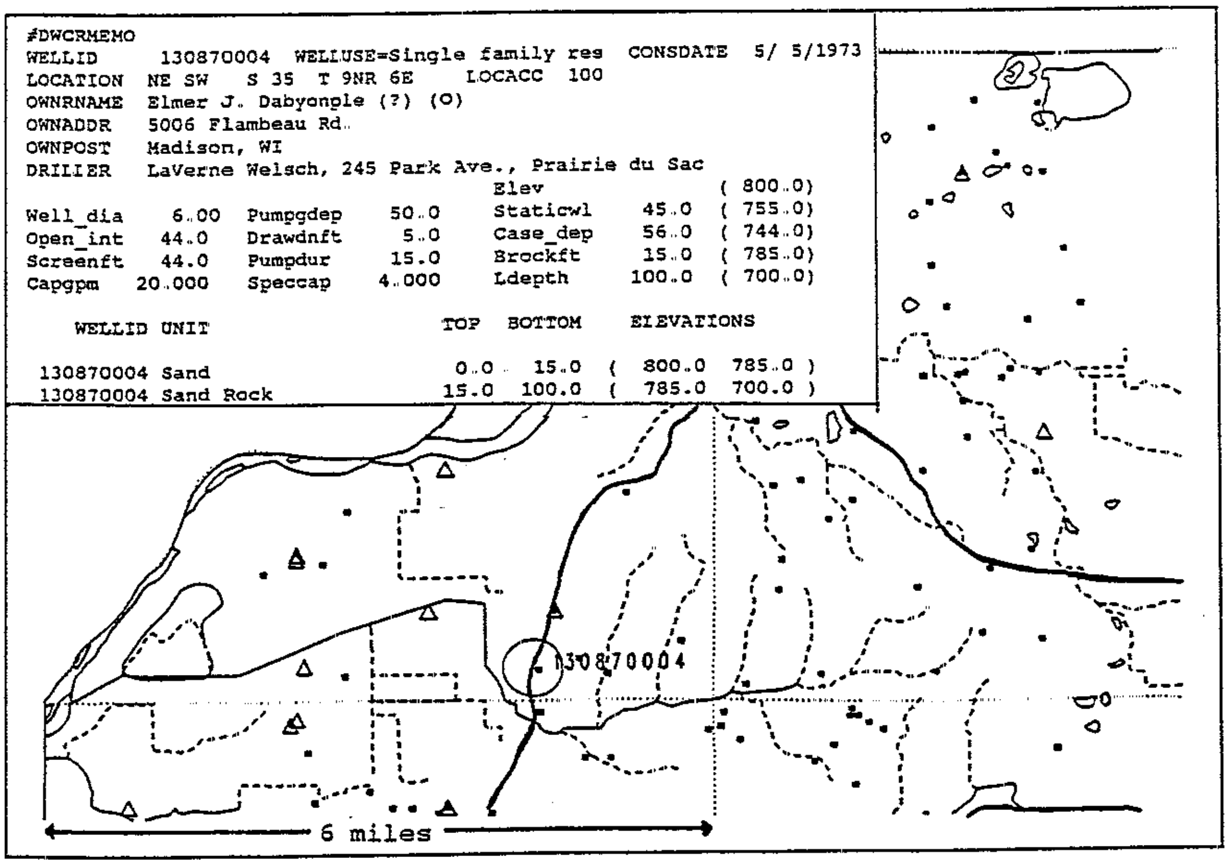


Figure 5. Pop-up screen with sample well constructor's report selected by user-defined circle. Δ indicates a well sampled for atrazine. ▪ indicates a well with a constructor's report. Heavy lines indicate roads, lighter lines are streams, and dashed lines are intermittent streams.

hydraulic conductivity and transmissivity, and displays the results to a pop-up screen. An example of the TGUESS output is shown in Figure 6. Hydraulic conductivity can be easily estimated from existing well constructor's reports (WCR_TGUESS) and that value assigned to an adjacent well that has been sampled for atrazine (TGUESS_2_WQ). PRETRAC also performs a unit conversion. TGUESS calculates hydraulic conductivity in units of ft/sec; when an operator assigns the hydraulic conductivity value to a sampled well, the hydraulic conductivity is converted to meters/day and the aquifer thickness is converted from feet to meters.

Of the 397 wells with atrazine sampling results, we could identify matching well constructor's reports for only about half. For sampled wells with matching constructor's reports, we used the hydraulic conductivity value calculated for the specific well after checking it against surrounding wells to insure that it was a reasonable estimate. For sampled wells with no constructor's report, we estimated aquifer parameters from surrounding wells. Typically constructor's reports were examined for 4 to 8 surrounding wells. We determined the elevation at which most wells were completed and then used the geometric mean *hydraulic conductivity for wells completed at that interval.*

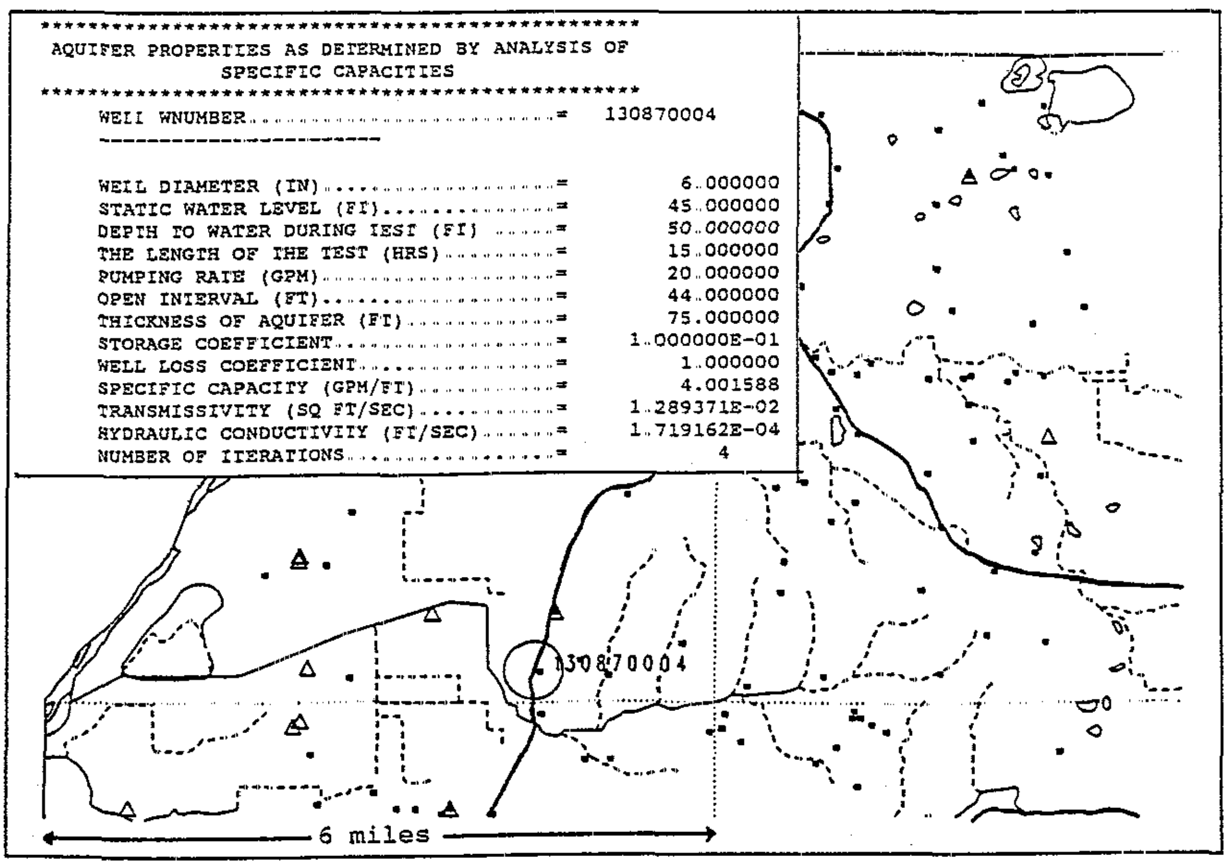


Figure 6. Example of TGUESS output. Parameters used in TGUESS calculation are pulled from WCR database.

The TGUESS program requires estimates of aquifer thickness, storage coefficient, and well loss coefficient. Since domestic wells frequently penetrate more than one lithologic unit (*i.e.*, interbedded sandstone, shale, and limestone or dolomite), we could not easily estimate aquifer thickness as the saturated thickness of any given lithologic layer. Further, it did not seem reasonable to use the entire saturated thickness of the Paleozoic section (from the Precambrian basement to the water table) as an aquifer thickness since domestic wells typically pump at a low rate and do not stress this entire thickness. In order to assess the importance of aquifer thickness and storage coefficient to the TGUESS estimation procedure, we varied these parameters for a bedrock well and a sand and gravel well located on the Black Earth quadrangle and compared the resulting hydraulic conductivity values. Results of this comparison are listed in Table 4. The second column lists aquifer thicknesses and the third and fourth columns show calculated hydraulic conductivity values (K) for a given storage coefficient (s). For each storage coefficient, calculated hydraulic conductivities for a given well are quite similar even as aquifer thickness was changed by more than 300 ft for the bedrock well and approximately 150 ft for the sand and gravel well. Comparison of columns 3 and 4 indicates that the calculated hydraulic conductivities for a given aquifer thickness do not vary significantly as the storage coefficient is changed from 0.1 to 0.01. This analysis suggests that the TGUESS algorithm is relatively insensitive to estimates of aquifer thickness and storage coefficient. For all subsequent TGUESS calculations we assumed an aquifer thickness that was equal to the saturated thickness of open interval of the well plus 50 ft, a storage coefficient of 0.1, and a well loss coefficient of 1. We felt that most domestic wells, which pump intermittently and at low rates (typically less than 15 GPM), would draw the majority of their water from the open interval and that this was the zone that was stressed by the specific capacity tests. The additional 50 ft added for aquifer thickness was meant to account for the fact that some water is drawn from above or below the open interval.

Table 4. Sensitivity of TGUESS estimated hydraulic conductivity to aquifer thickness and storage coefficient variability.

Well	Aquifer thickness (ft)	(s=0.1) K (ft/sec)	(s=0.01) K (ft/sec)
871010	68 (open int +50 ft)	3.24×10^{-4}	3.47×10^{-4}
(bedrock)	250 (WT to well bottom)	3.26×10^{-4}	3.32×10^{-4}
	400 (est. sandstone)	3.42×10^{-4}	3.46×10^{-4}
871065	56 (open int +50 ft)	1.55×10^{-3}	1.61×10^{-3}
(sand &	80 (saturated s & g)	1.58×10^{-3}	1.62×10^{-3}
gravel)	400 (s & g and est sandstone)	1.79×10^{-3}	1.81×10^{-3}

Porosity

GPTRAC requires an estimate of the porosity for the units penetrated by the sampled well. Ranges of porosity values summarized by Freeze and Cherry (1979, p. 37) were used to develop estimated porosities for a variety of lithologic units: sand and gravel, 30%; sandstone, 25%; shale, 20%; and limestone, 10%. For sampled wells with a matching constructor's report, porosities were estimated for the saturated units penetrated by the open interval of the well. If a well penetrated more than one lithologic unit, a thickness-weighted porosity was calculated. For sampled wells without a matching constructor's report, thickness-weighted porosities were calculated for the wells that had been used to calculate hydraulic conductivity and the average porosity calculated from surrounding wells was assigned to the sampled well using the EDITWQ menu choice.

After aquifer parameters had been determined for all sampled wells on a given topographic quadrangle map, the modeler could select those wells (SEL_4_GPT) and write out individual input files (DUMPGPT) that were then used in the particle-tracking model.

GPTRAC Modeling

We ran the GPTRAC model in the numerical mode. The hydraulic head data files were derived from the 1:100,000-scale water-table map. The model has a maximum grid size of 55 columns and 55 rows. We chose a uniform node size of approximately 250 m^2 and a model grid of 41 columns and 55 rows. This allowed us to model an area the size of a 1:24,000-scale topographic quadrangle map. Hydraulic conductivity, aquifer thickness, and porosity were determined for each sampled well.

GPTRAC tracks particles for a user-specified time period. We chose to run the model for a 15 year time period for the following reasons. Atrazine has been used for approximately 30 years, however, we had land-use information for only 12 years (see Chapter 4). The site-specific research projects conducted by Chesters and others (1991) and Bradbury and McGrath (1992) suggest that the majority of atrazine contamination at those sites has occurred in the last 10 to 20 years. In addition, the 15-year travel times generated ZOCs of reasonable size over most of the county.

The model can calculate ZOCs by one of two methods. If the user specifies that a ZOC should be calculated for a pumping well, the model will place 10 particles around the well and then use the entered pumping rate to move the particles out of the first node. After the particles reach the node boundary, they are tracked according to the hydraulic gradient and pumping is no longer used in the iteration technique. We encountered problems with this solution technique due to the low pumping rates of domestic wells. In some cases the 15-year travel time was not long enough to track the particle out of the pumping node and as a result no ZOC was calculated. The other method of calculating ZOCs requires that the user place particles around the well and then specify that the model not calculate a ZOC for the pumping well. In this case the model just moves the particles according to the hydraulic gradient. We used this method to calculate ZOCs. We placed 8 particles in a circle around the well; the circle had a radius of 50 meters. By using this method, we predetermined the width of the ZOC at the wellhead. We felt that this was an adequate width for the ZOC at the wellhead because it is unlikely that a domestic well pumping at low rates would develop a drawdown cone that was more than 100 meters in diameter.

We calculated 15-year capture zones for each of the 397 sampled wells. Figure 7 shows calculated ZOCs for four wells in a small sub-watershed in western Dane County. The model produces eight pathlines, one for each particle. A boundary was hand-drawn around the particle pathlines. This boundary was digitized and given to the Dane County LCD. They identified agricultural land uses by delineating the fields contained within the ZOC for a given well and interpreting the field cropping histories for the previous 12 years. This process is explained more fully in the following chapter.

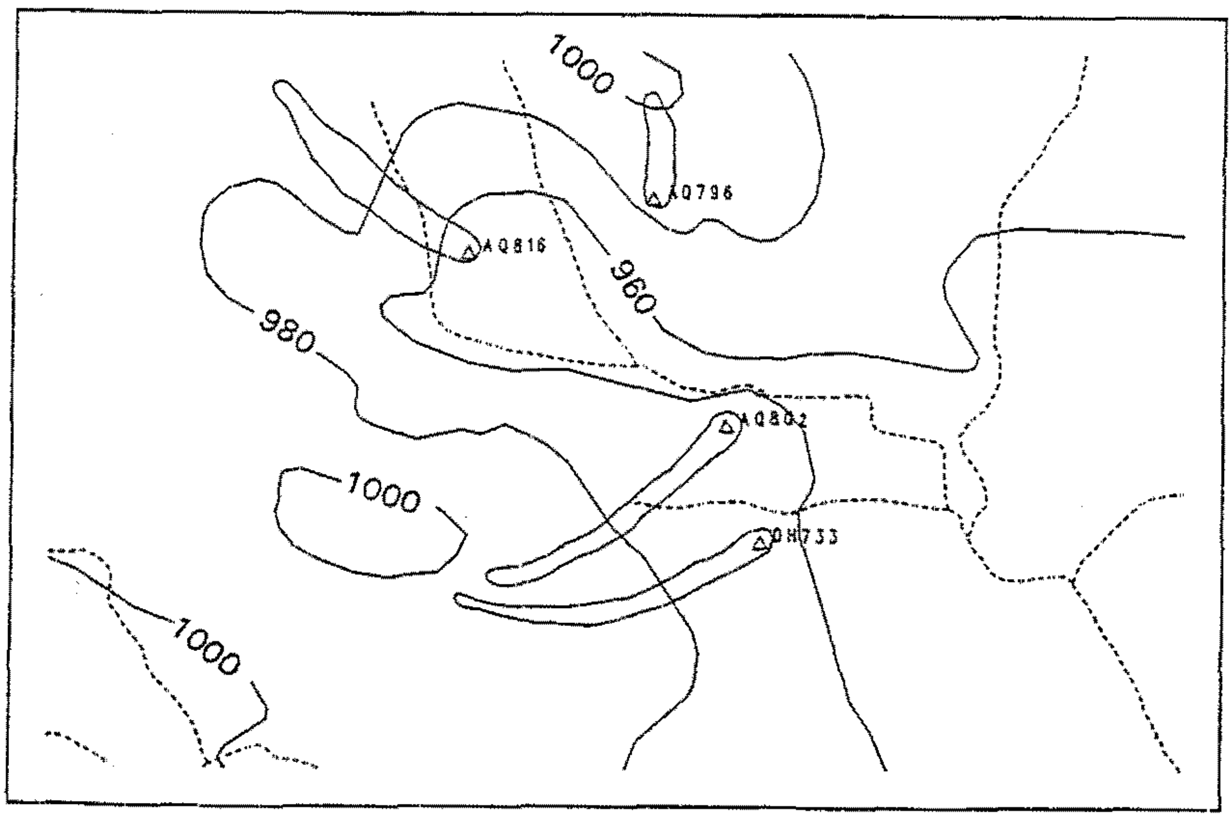


Figure 7. Water-table map and calculated ZOCs for a small sub-watershed in western Dane County. Distance across map is approximately 2 miles.

Chapter IV.

LAND-USE DETERMINATION

Determination of Cropping History

Personnel from the Dane County LCD used PC ARC/INFO to display 12 years of cropping history (1979 - 1990) for farm fields located within each of the 397 ZOCs. Rural land-use information was available in the tracts and fields coverages, which were digitized in 1988 by the LCD from 1:12,000-scale USDA Agricultural Stabilization and Conservation Service (ASCS) aerial photographs and transformed to the DaneTM coordinate system. The tracts and fields coverages contained boundaries of agricultural management units and other land types such as wooded areas or residential subdivisions. These boundary coverages were spatially overlaid with coverages containing ZOC boundaries created at WGNHS, resulting in new coverages for the areas of intersection. This process created 'ZOC/field boundary coverages' that divided each ZOC into a number of smaller areas, each area corresponding to a different land-use type.

Two computers were required to perform the crop history analysis. The first computer controlled an optical disc player containing video images of the ASCS 35 mm crop compliance air photos for the twelve years from 1979 to 1990. The image retrieval system allowed users to retrieve the airphoto for any given section of land for any given year in a matter of a few seconds. The second computer had a "frame grabber" installed, allowing the images on the optical disc, (controlled by the first computer) to be displayed on the second computer's screen. This visually integrated the two sources of information, allowing the air photos to be seen as a backdrop while using PC ARCEDIT to enter and edit crop histories for the ZOC/fields boundary coverages. This two-computer system also has the capability to update field boundaries. If an operator finds field polygons delineated on the video images that are not delineated in the ZOC/field boundary coverages, they can use on-screen digitizing to enter the new boundaries and interpret the crop history in the new areas.

Macros written in PC ARC/INFO's Simple Macro Language facilitated the air photo interpretation and editing operations in ARCEDIT. Land uses were interpreted for each field in each ZOC for each of the twelve years. A character code (Crophist) representing the land use was then assigned to each field for each year. As shown in Table 5, the codes "CCCCHHHHCCCC", represents four years of corn (from 1979-1982), four years of hay (1983-1986) and four years of corn (1987-1990).

Estimate of Atrazine Usage

Experts familiar with Dane County agricultural practices who had experience in herbicide application estimated typical application rates of atrazine for a variety of crops.

Atrazine is primarily applied to corn and sorghum fields. The other crops listed in Table 5 (vegetables, tobacco, etc) do not receive atrazine applications. Since many dairy operations rely on a corn-oats-hay crop rotation, we wanted to account for differences in atrazine application rates due to these rotations. The effect of the crops grown in preceding and subsequent years was codified into a set of rules shown in Table 6. These estimation rules were coded into a FORTRAN computer program and used to compute atrazine application rate estimates for fields in each ZOC.

Table 5. Photo-interpreted crop types and abbreviations.

Code	Crop Type	Code	Crop Type
B	Beans - soy and snap beans	P	Peas
C	Corn, incl. feed, seed, and sweet corn	R	Railroad right-of-way
D	Developed - farmstead, etc.	S	Sorghum
F	Forest	T	Tobacco
H	Hay, alfalfa, meadow	U	Unidentifiable (but not corn)
K	Potatoes	V	Vegetables and fruits
M	Mint	W	Winter wheat
O	Oats	Z	Strip cropping

Table 6. Atrazine application rate estimates.

Code	Crop type	Atrazine application **
C	Corn, incl. feed, seed, and sweet corn	1.8 lb/acre/year
S	Sorghum	0.8 lb/acre/year
Z	Strip cropping *	0.8 lb/acre/year
R	Railroad right-of-way	5.0 lb/acre/year

* Strip crop, a mixture of hay and corn, was calculated as 6 years of hay and 6 years of corn, 2 with heavy application of atrazine, 2 with medium application, 2 with no application. Average to 0.8 lbs/acre/year.

** Crop rotations are an important factor in atrazine use. The influence of crops grown in preceding or subsequent years was estimated. The application rates for corn and sorghum were modified for each year based on the sequential application of the following rules:

1. If continuous corn for all years, the rate is 3 lbs/acre.
2. If a year of corn is followed by corn, and is preceded by 3 or fewer years of hay, the rate is 3 lbs/acre.
3. If a year of corn is followed by corn, and is preceded by 4 or more years of hay, the rate is 5 lbs/acre.
4. If corn is followed by oats or hay, the rate is 0.8 lbs/acre.
5. If a year of corn is both preceded and followed by non-atrazine tolerant crops, the rate is 0.8 lbs/acre.

Chapter V.

STATISTICAL ANALYSIS

The movement of agricultural chemicals from the ground surface to a domestic well is governed by a variety of processes. Atrazine applied on a given field may degrade *in-situ*, run off to surface water, move by means of soil erosion to lower points in the landscape, or infiltrate to the unsaturated zone. In the unsaturated zone, physical and biological processes may decrease the concentrations of parent atrazine as well as metabolites. After atrazine or its metabolites reach the water table, little attenuation or degradation occurs; concentrations may decrease by dilution, Chesters and others (1991, p. 118). In the saturated zone, the distribution of atrazine is controlled primarily by groundwater advection and so variations in groundwater flow paths are important in predicting which wells may contain the pesticide.

The physical and biological processes controlling atrazine degradation and attenuation in natural systems are not fully understood. One of the primary goals of this study was to determine which soils, geologic, and hydrogeologic factors are important in controlling the distribution of atrazine detections in domestic wells. To this end, we developed several variables to characterize various aspects of the physical system, as well as the land-use history and well construction. Given the large number and wide variety of variables that we needed to consider, we explored many statistical tools to look for patterns within the data. Statistical analysis consisted of an iterative process of data exploration, development of descriptive statistics, stratification of the dataset into sub-populations, and examination of the relationships between various sub-populations and the pattern of atrazine detections. With each iteration we identified wells that we felt should be excluded from further analysis, developed additional variables, categorized existing variables in new ways, and further refined our stratification of the dataset into meaningful sub-populations. The following sections summarize this process and the results.

Choice of Variables

A variety of models have been developed to assess the vulnerability of aquifers to pesticide contamination (U.S. EPA, 1990) and each model uses a slightly different combination of variables to assess differing hydrogeologic, climatic, and land-use characteristics. We reviewed several of these models to determine which variables other workers had found useful in assessing aquifer sensitivity to contamination. Parameter-weighting models and empirical statistical models helped identify key variables.

Parameter weighting models, such as *DRASTIC* (Aller and others, 1985) and the Wisconsin *Groundwater Contamination Susceptibility* map (DNR and WGNHS, 1989) include information on various aspects of the hydrogeologic system. Specifically, *DRASTIC* considers depth to water table, net water recharge, soil material, unsaturated zone thickness, aquifer material, aquifer hydraulic conductivity, and topography. The Wisconsin model considers type and depth of surficial materials, type and depth of bedrock, and depth to water table. Both of these models have been developed by panels of experts and incorporate their understanding of the physical processes involved in contaminant movement into subjective weighting schemes. Specific water-quality data are not incorporated into the development of these models.

Several Midwestern states have conducted sampling programs to determine the extent of contamination of domestic wells by agricultural chemicals and to evaluate which settings are most susceptible to contamination (for example Kross and others, 1990, Schock and Mehnert, 1991). In addition to these efforts, a few statistical studies conducted at a more local scale have tried to develop empirical relationships between pesticide detections and various physical and land-use factors. The advantage of these studies is that water-quality data from a given area have been used to determine which factors are most responsible for pesticide detections. Teso and others (1988) used discriminant analysis with soil classification data to predict sites of existing and potential contamination. A study in Nebraska determined that the following parameters were important in predicting variations in atrazine concentrations at six study sites: hydraulic conductivity of the unsaturated zone, specific conductance of well water, irrigation well density, pesticide application date, average screened well depth, and depth to water table (Chen and Druliner, 1987; and Druliner, 1989).

After reviewing the parameter-weighting susceptibility models, results from other states' sampling programs, and statistical studies conducted at more local scales; we decided we would consider five types of predictive variables in our analysis. These include: soils, geology, hydrogeology, well construction, and land use. These five types of variables were used as independent variables that might prove to be useful predictors of atrazine concentrations, the dependent variable. All of these variables are described in more detail in the following sections.

Data Exploration and Descriptive Statistics

Data exploration consisted of two processes; 1) the characterization of variables in terms of descriptive statistics and 2) the use of PRETRAC to examine load and concentration data in relation to ZOC boundaries, water-table map, SCAM2 rankings, bedrock geology, and well constructor's reports.

Descriptive Statistics

Variables used in our analysis are categorized as soils, geologic, hydrogeologic, well construction, land use, and atrazine concentrations. Each variable is described in the following "Description of Variables" section. Many of the variables within the six categories are treated as both discrete and continuous variables. Continuous variables, such as depth to water table, are described by a variety of statistical measures. The first step in our data exploration process was to examine the distribution of all of our continuous variables by generating histograms and calculating the standard statistical measures such as mean, median, standard deviation, skewness, and kurtosis. We used Kolmogorov-Smirnov and Chi-squared goodness-of-fit measures to determine whether a normal or log-normal distribution better described the data. For log-normal distributions we calculated a geometric mean; for normal distributions we calculated an arithmetic mean. We generated a table for each category of variables (Table 7 - soils, Table 8 - geologic, Table 9 - hydrogeologic, Table 10 - well construction, Table 11 - land use, and Table 12 - atrazine concentration). Statistical analysis was an iterative process and with each iteration we identified wells that we felt should be excluded from further analysis. After starting with 397 wells we chose to conduct our analysis using 325 wells. Tables 7, 8, 9, 11, and 12 reflect the summary statistics for the population of 325 wells; Table 10, well construction, summarizes statistics for the 137 wells for which we had WCRs. An explanation of which wells were excluded from analysis follows the "Description of Variables" section.

Discrete variables include yes/no flags or simple numeric codes. Sample statistics for these variables are simple counts of the number of values falling into each category. Several of our variables can only be treated as discrete variables, for example atrazine detection vs. no detection. Very few statistical tests are able to compare discrete to continuous variables. Several non-parametric techniques have been developed to analyze discrete variables. To utilize all of our data in these tests, we divided the continuous variables into categories that were generally based on the quartiles of distribution. Summary statistics for these discrete variables are also included in Tables 7 to 12.

Spatial Exploration of Data

To assess the spatial variability of the physical and land-use characteristics, we used PRETRAC to examine load and concentration data in relation to ZOC boundaries, water-table map, SCAM2 rankings, bedrock geology, and WCRs. We started with the assumption that high loads would lead to a greater percentage of detections and detections at higher concentrations. By noting exceptions to this trend, we identified general variables that we thought were important in controlling atrazine detections and identified some sub-populations of wells that did not fit the general trend.

<u>Additional categorization of variables</u> - Spatial exploration of the data suggested that application rate, position in flow system, presence of shale, and casing depth (for a limited number of cases) are important variables for predicting atrazine detections. The general trend of increasing load leading to more detections was not as strong for 1) discharge wells (excluding those discharge wells located in the Wisconsin River Valley), 2) ZOCs that contained shale, or 3) ZOCs in the southwest portion of the county that had Sinnipee Group dolomite as the uppermost bedrock unit over a majority of the ZOC. We developed codes to identify wells in the Wisconsin River Valley (Table 9) and ZOCs in the southwest portion of the county with Sinnipee Group dolomite (Table 8). These sub-populations are described more fully in the "Results" section later in this chapter.

Description of Variables

Soils

The processes controlling attenuation and degradation of atrazine are not fully understood, however, it is known that little degradation occurs once the pesticide reaches the water table (Chesters and others, 1991). This suggests that the soil column (upper 5 ft of unlithified material at the earth's surface), is the location of many attenuation processes. We chose to use three variables to describe various features of the soil column (see Table 7).

Table 7. Descriptive statistics for soil variables.*

	Arithmetic Mean	*Median*	*Std dev*	*Minimum*	*Maximum*	Distrib**
Soil thickness (inches)	35.1	34.0	12.4	5.0	65.0	N
Category	*Frequency*	*Percent*				
≤ 6	1	.3				
7 - 18	42	12.9				
19 - 30	51	15.7				
31 - 42	139	42.8				
43 - 54	75	23.1				
> 54	17	5.2				
Area-weighted silt thickness (inches)	19.9	20.6	10.6	0.0	48.5	N
Category	*Frequency*	*Percent*				
0 - 13.9	95	29.2				
14 - 21.2	75	23.1				
21.3 - 27.3	76	23.4				
27.4 - >	79	24.3				
Area-weighted SCAM2 score	42.5	44.4	8.4	16.0	53.9	O
Category	*Frequency*	*Percent*				
Least [0-30]	32	9.8				
Marginal [31-40]	83	25.5				
Good [41-50]	149	45.8				
Best [>50]	61	18.8				

*Each variable is listed in bold type followed by the descriptive statistics for the continuous variable (arithmetic mean, median, standard deviation, minimum, maximum and description of distribution). If the variable was also treated as a discrete variable, the categories are listed on subsequent lines, along with the frequency and percent occurrence.

** N=Normal Distribution, L=Log-Normal, O=Other

Soil thickness - The SOIL5 database describes the range of typical thickness for each soil map unit. Soils can be anywhere from 5 to 60 inches thick. In some places the depth to bedrock controls soil thickness; in places with more than 5 feet of unlithified material, soil depth is determined by the depth to which soil forming processes have altered the parent material. We determined soil thickness at the point location of the well. Soil thicknesses were categorized as $\leq$ 6 inches, 7-18", 19-30", 31-42", 43-54", and > 54 inches (Table 7).

Silt thickness - Soils in Dane County, both in the glaciated and unglaciated areas, are developed in silt of varying thickness which overlies other materials (see Chapter 2). Silt thickness of each soil map unit was interpreted from the *Soil Survey of Dane County* (Glocker and Patzer, 1978). This information was linked to the digital soils coverage by a lookup table. An area-weighted average silt thickness was determined for each ZOC. We used the quartiles of the distribution to develop categories of silt thickness (Table 7).

SCAM2 ranking - The SCAM2 model uses physical and chemical characteristics of soil series to evaluate "the ability of the soil solum (the A and B horizons) to attenuate potential contamination resulting from activities above or within the soil zone" (Cates and Madison, 1990). Within each ZOC, we calculated SCAM2 rankings for each soil map unit. As a general measure of the ZOC's ability to attenuate contaminants, we calculated the area-weighted average SCAM2 ranking. These area-weighted average SCAM2 rankings were categorized according to the divisions for least, marginal, good, and best ability to attenuate contaminants (Table 7).

Geologic

Most workers assume that different geologic settings will have differing susceptibility to contamination (U.S. EPA, 1990). One of the reasons Dane County was chosen as a project area was its diversity of geologic settings. However, this diversity presented several challenges for our statistical analysis. We developed numerous variables to characterize the geologic features that we thought might be controlling atrazine movement. These variables included simple yes/no flags as well as more complicated codes that attempted to characterize the vertical variability of both the unlithified units and the bedrock units (see Table 8).

Glaciation flag - A simple flag indicating if the ZOC was in the glaciated or unglaciated portion of the county.

Depth to bedrock - We did not try to develop a depth-to-bedrock variable that would characterize the entire ZOC, rather we determined depth-to-bedrock at the point location of the well. If a WCR was available for the sampled well, we determined depth to bedrock from the report. If no WCR was available, we estimated depth to bedrock from the depth-to-bedrock coverage described in Chapter 2. The depth-to-bedrock categories in Table 8 are subjective divisions that reflect the sources of our data. The depth-to-bedrock map has a 50-ft contour interval and the Soil Survey indicates areas where bedrock is within 5 feet of the land surface.

Unlithified material - The type of unlithified material at the point location of the well was determined from the soil parent material coverage (described in Chapter 2). In places where the depth to bedrock was more than 10 feet, we thought that the uppermost material might not represent the majority of the unlithified materials. In order to simplify the analysis, we assumed that till and outwash tend to be thick continuous units whereas silts, lacustrine deposits, and organic deposits are generally not as thick nor as continuous. For these thinner units, we examined each case individually and assigned an unlithified material code (either till, outwash, or silts) that best represented the majority of the underlying material. Choice of code was based on the well's position in the landscape and information from nearby WCRs.

Unlithified material categories were further aggregated into coarse-grained materials (outwash and till) or predominantly fine-grained materials (silts and weathered bedrock).

Bedrock - Most workers agree that the type of bedrock can be an important control on the movement of contaminants into the groundwater system. In Dane County, over 90% of domestic wells are completed in bedrock aquifers. We felt that we needed to develop variables describing bedrock at the point location of the well and over the entire area of the ZOC. Variables determined at the point location of the well include uppermost bedrock formation and the environment of deposition of uppermost bedrock formation. For the entire ZOC, we developed flags indicating whether shale or thick clay was present or whether the majority of the ZOC had Sinnipee Group dolomite as the uppermost bedrock unit (for wells in the unglaciated area).

Bedrock variables determined at location of well - Statistical analysis of the wide range of geologic settings in Dane County required that we develop a systematic method of aggregating similar geologic units. We chose to characterize the geologic formations in terms of depositional environment. Ostrom (1965) has suggested that four major depositional environments have repeated themselves five times in southern Wisconsin, each time depositing a characteristic sequence of rock types. Each cycle begins on an erosional surface. The deposition sequence starts with a nearshore-beach setting (1) characterized by slow to rapid subsidence with heavy sediment loads; clean sandstones are deposited. This is followed by a non-depositional shelf setting (2), a characteristically low subsidence, high-energy environment where previously deposited sediments are ripped up and reworked; poorly-sorted sandstones are the characteristic rock type. This is followed by depositional shelf environment (3); more rapid subsidence with low sediment loads results in shaley, argillaceous sandstones. The sequence is capped with reef/inter-reef deposits (4); in this environment low sediment loads lead to carbonate formation.

The four depositional environments, coded 1 to 4, were used to characterize the vertical sequence of bedrock units at the point location of the sampled well. If a WCR was available, rock types and thicknesses were determined directly from the report. If a WCR was not available, information from nearby WCRs and from the digital bedrock coverage was used to develop a "representative log" for the sampled well. Since most wells penetrate

Table 8. Descriptive statistics for geologic variables.

	Geometric Mean	Median	Minimum	Maximum	Distrib*
Glaciation Flag					
Category	*Frequency*	*Percent*			
Not glaciated	121	37.2			
Glaciated	204	62.8			
Depth to Bedrock (feet)	31.0	42.0	0.0	239.0	L
Category	*Frequency*	*Percent*			
0-5	49	15.1			
6-10	37	11.4			
11-50	100	30.8			
51-100	90	27.7			
>100	49	15.1			
Unlithified materials					
Category	*Frequency*	*Percent*			
Coarse-grained					
Outwash	86	26.5			
Till	143	44.0			
	229	70.5			
Fine-grained					
Silts	21	6.5			
Weathered Dolomite	43	13.2			
Weathered SS/Shale	6	1.8			
Weathered Sandstone	26	8.0			
	96	29.5			
Environment of deposition for uppermost bedrock unit					
Category	*Frequency*	*Percent*			
Beach - sandstone (1)	119	36.6			
Non-depositional shelf (2)	0	0.0			
Offshore - shaley sandstone (3)	33	10.2			
Reef - carbonates (4)	149	45.8			
Sand & Gravel (5)	24	7.4			
Presence of shale or thick clay					
Category	*Frequency*	*Percent*			
shale/clay reported in WCR	33	10.2			
shale/clay inferred	52	16.0			
no shale or clay	240	73.8			
Sinnipee Group Dolomite					
Category	*Frequency*	*Percent*			
Not Sinnipee	276	84.9			
Sinnipee	49	15.1			

* L=Log-normal distribution

several bedrock units, we needed to further simplify our bedrock data. For each well we analyzed only the uppermost bedrock formation and the depositional environment of the uppermost bedrock formation (coded 1 to 4). Wells that do not reach bedrock were coded as sand and gravel (5).

Bedrock variables determined over entire ZOC - In many cases, parts of the ZOC encompassed a different stratigraphic sequence than that penetrated by the well. This is especially common in the unglaciated portion of the county where wells are frequently located in valleys and ZOCs extend to upland areas. Water recharging anywhere within the ZOC has the potential to move to the well, therefore, it was important to characterize some aspects of the stratigraphic sequence for the entire ZOC. One of the factors we chose to examine was presence or absence of shale or thick clay.

The only mapped shale unit in Dane County is the Maquoketa shale and its distribution is limited. Many of the sandstone formations contain shale interbeds; unfortunately these shales are not always laterally continuous. As a result it is difficult to determine the presence/absence of shale by examining the bedrock geology map in conjunction with the stratigraphic column. To determine if shale underlay any portion of the ZOC, we plotted over 3000 WCR data points that indicated if "shale" appeared in the driller's description of the geologic units. The ZOC boundaries and the WCR points were overlain on the bedrock geology map and we made determinations for each ZOC as to whether it was likely that shale was present. While examining the individual ZOCs we also determined if thick clay sequences were present in the unlithified materials. Codes indicated no shale or clay (0), shale or clay confirmed from WCR (1), or shale or clay inferred from surrounding WCRs and geologic map (2).

Exploration of the atrazine data using PRETRAC indicated that the general trend of increasing load leading to more detections was not as strong for ZOCs in the southwest portion of the county that had Sinnipee Group dolomite as the uppermost bedrock unit over a majority of the ZOC. Figure 8 shows the glaciated and unglaciated portions of the county along with the generalized area where Sinnipee Group dolomite is the uppermost bedrock unit. This boundary was generalized from the digital bedrock geology map for Dane County. We were primarily interested in determining which ZOCs had the Sinnipee as the uppermost unit; so the generalized area in Figure 8 includes some areas where the Sinnipee is not the uppermost unit (for example valleys) and excludes other areas where the Sinnipee is the uppermost unit (for example ridgetops with no ZOCs).

Hydrogeologic

<u>Flow system position</u> - In unconfined aquifers, groundwater movement is primarily from upland recharge areas to low-lying discharge areas. Recharge areas are characterized by net downward flow of groundwater while discharge areas are characterized by net upward flow. In the middle portion of flow systems, flow is primarily horizontal. Our ZOC determinations are based on the assumption of two-dimensional groundwater flow.

Inaccuracies in ZOC determinations limit all other aspects of the statistical analysis; we assume that the delineated ZOC is the land area that supplies water to the well and we then determine the land-use and physical characteristics of that ZOC area.

The assumption of two-dimensional groundwater flow is not valid in recharge and discharge areas. Nonetheless, we believe that the delineated ZOC in a recharge area is a reasonable estimate of the land area supplying water to the well because ZOC size is limited by a nearby groundwater divide and water movement is primarily downward. In essence there's really nowhere else for the water to originate. The physical and land-use characteristics determined for the ZOC should be reasonable predictors of water quality in the sampled well. In discharge areas, it is likely that water reaching domestic wells is traveling along deeper, more regional flow paths. In this case, the land area supplying water

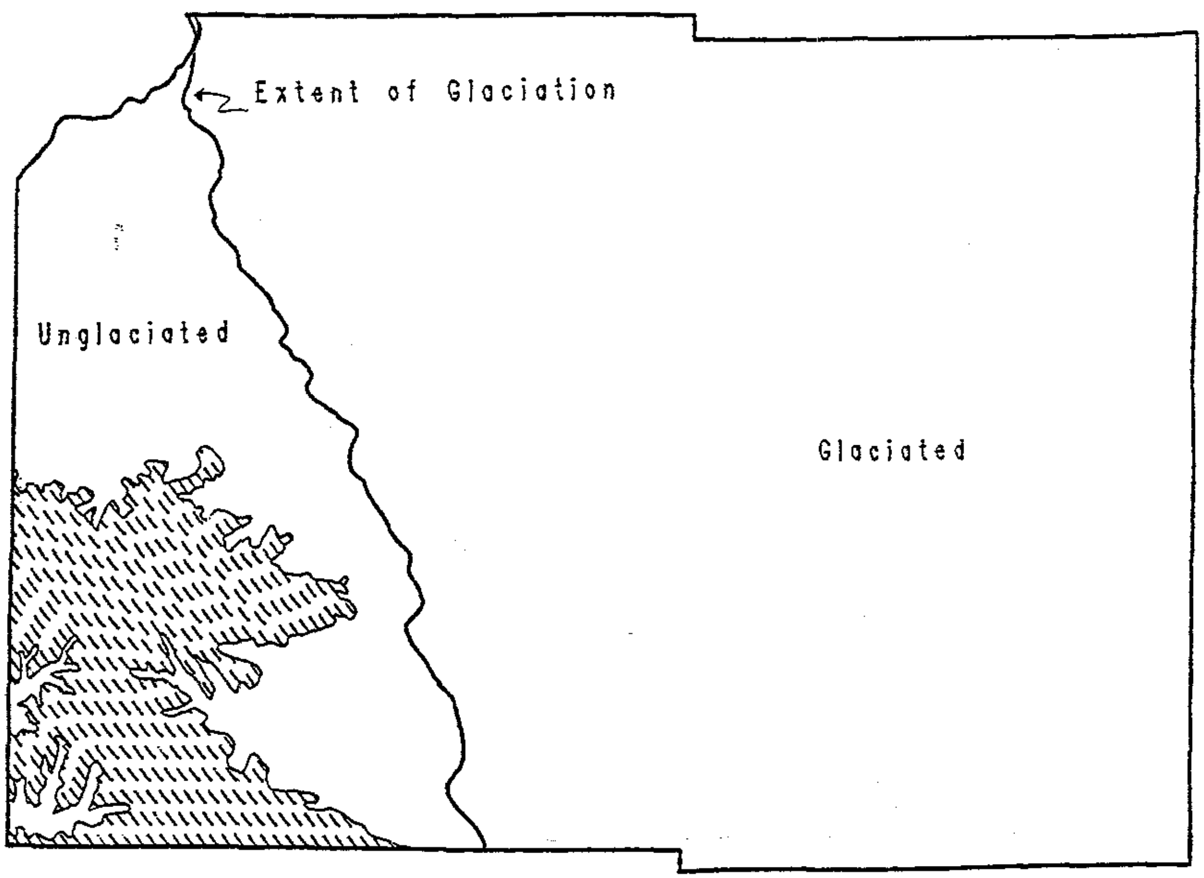


Figure 8. Map showing general area where ZOCs had Sinnipee Group dolomite as uppermost bedrock unit.

Table 9. Descriptive statistics for hydrogeologic variables.

	Geometric Mean	Median	Minimum	Maximum	Distrib*
Flow system position					
Category	*Frequency*	*Percent*			
Recharge area	57	17.5			
In between	196	60.3			
Discharge area	72	22.2			
*Confidence in ZOC***					
Category	*Frequency*	*Percent*			
High	223	68.6			
Medium	102	31.4			
Depth to water table (ft)	40.8	40.0	1.0	314.0	L
Category	*Frequency*	*Percent*			
0-20	76	23.4			
20-40	94	28.9			
40-80	72	22.2			
80-160	60	18.5			
>160	23	7.1			
Unlithified vadose thickness (ft)	14.4	14.0	0.0	180.0	L
Category	*Frequency*	*Percent*			
0	24	7.4			
1-5	59	18.2			
6-10	48	14.8			
11-25	91	28.0			
26-50	76	23.4			
>50	27	8.3			
Bedrock vadose thickness (ft)	42.0	8.0	0.0	304.0	L
Category	*Frequency*	*Percent*			
0	150	46.2			
1-20	37	11.4			
21-40	49	15.1			
41-100	41	12.6			
>100	48	14.8			
Wisconsin River Valley					
Category	*Frequency*	*Percent*			
Located in WI River Valley	13	4.0			

* L=Log-normal distribution

** Wells for which we had low confidence in the delineated ZOC were excluded from the analysis.

to the well is probably larger than the delineated ZOC. The physical and land-use characteristics determined for the ZOC will not be good predictors of the water quality in the sampled well. For wells in the middle of flow paths, the assumption of two-dimensional groundwater flow is more likely to be valid and we assume that the delineated ZOC is a close approximation of the land area that actually supplies water to the well.

Dane County can be divided into five groundwater basins (see Chapter 1) separated by regional groundwater divides. For each sampled well, we determined the position in the flow system by overlaying the delineated ZOC boundaries on the digitized water-table map and coding each well as recharge, middle, or discharge (see Table 9). Recharge and discharge delineations were based on regional flow systems rather that local flow systems; ZOCs located near regional divides were coded as recharge and wells located in major stream valleys or near large lakes were coded discharge. The majority of ZOCs were in the middle of flow paths.

Confidence in determination of ZOC - A flag indicating our confidence in the delineated ZOC boundaries incorporates subjective estimates of the accuracy of both flow-direction determinations and hydraulic conductivity estimates. The shape and orientation of the ZOCs delineated with GPTRAC depend primarily on the configuration of the water table and how well the water-table configuration is captured by the gridded values of hydraulic head (see Chapter 3). Confidence in our determination of groundwater flow direction, and hence ZOC orientation, is highest in areas of steep water-table gradient and lowest in low-gradient areas.

The size of the delineated ZOC depends on the velocity of the particles tracked by GPTRAC. Groundwater flow velocity depends both on hydraulic gradient and hydraulic conductivity. Methods used to estimate hydraulic conductivity are outlined in Chapter 3. GPTRAC has the capability of incorporating spatial variations in hydraulic conductivity, however, we did not feel that we had adequate data to describe these variations and we assumed that the hydraulic conductivity calculated for each sampled well was uniform over the model area. In some cases, low hydraulic conductivity values resulted in exceedingly small ZOCs; in general, we had only medium confidence in these ZOCs.

ZOC boundaries serve as the basis of our estimates of atrazine loads. We tried to incorporate this fact into our estimate of ZOC confidence. For example, in some areas we may have only had low confidence in our determination of flow direction and hence ZOC orientation, however, if this entire area exhibited similar land-use patterns, then our estimate of atrazine load would not change much even if the ZOC orientation shifted. For these cases we assigned the ZOC a medium confidence.

Confidence in ZOC delineation was coded high, medium, or low for each sampled well (see Table 9). This determination was primarily based on an estimation of water-table map accuracy and how well we could determine flow-system direction, however, estimates of hydraulic conductivity and the consistency of surrounding land-use were used as secondary considerations.

Depth to water table - Depth to water table was calculated by subtracting water-table elevations from land-surface elevations for each of the 325 wells (see Table 9). Water-table elevations were determined at the point location of the well by visually interpolating the position of each well between 20-ft water-table contours. Land surface elevations were estimated from visually interpolating the position of each well between the 7.5' topographic quadrangle elevation contours with either 10-ft or 20-ft contour intervals. The first four categories in Table 9 are approximately based on the quartiles of the log-normal distribution; the upper quartile was divided at approximately the 90th percentile to create the 80-160 and >160 ft categories.

Thickness of geologic materials in vadose zone - The Wisconsin model of assessing groundwater vulnerability (DNR and WGNHS, 1987) assumes that depth to the water table and type of material in the unsaturated zone are important variables in determining vulnerability. We developed two variables that combine depth-to-bedrock information with information concerning thickness of the vadose zone. Vadose zone thickness was calculated as depth to water table minus soil thickness. All variables were determined at the point location of the well; calculated variables include thickness of unlithified material in the vadose zone and thickness of bedrock material in the vadose zone. The categories in Table 9 are roughly based on the quartiles of the log-normal distribution.

Well Construction

Other studies have indicated that well construction can play an important role in determining whether pesticides contaminate in domestic wells (Hallberg and others, 1992; Schock and Mehnert, 1991). We identified WCRs for 137 or approximately 42% of the 325 wells included in the statistical analysis. We chose to look at total well depth and casing depth, as well as casing depth in relation to water-table depth. Statistics describing these variables are summarized in Table 10. Categories for well depth and casing depth relative to water table are approximately based on the quartiles of the log-normal distribution.

Land use

Methods used to delineate land-use patterns, determine cropping histories, and estimate atrazine usage are outlined in Chapter 4. At the end of this analysis there were several estimated atrazine application rates for each ZOC since atrazine application rates had been determined for each field or portion of field for each of 12 years. In order to use the atrazine rate information in statistical analyses we needed to develop variables that integrated the atrazine-use information for the entire ZOC. Calculation of these values is not straightforward; application rates vary in time and vary spatially within each ZOC. We chose to look at loads as well as rates (see Table 11).

Total load - This value was calculated by multiplying the application rate for each field (lb/acre) times the area of the field (acres) and then summing these values for the 12 years that we have cropping history information. Units are pounds. This value of atrazine load

Table 10. Descriptive statistics for well-construction variables.

	Geometric Mean	Median	Minimum	Maximum	Distrib*
Well Depth (ft)	139.6	142.0	50.0	360.0	L
Category	*Frequency*	*Percent*			
0 -119	49	35.8			
120-149	22	16.1			
150-199	29	21.2			
200->	37	27.0			
Depth of casing (ft)	65.5	55.0	20.0	239.0	L
Category	*Frequency*	*Percent*			
<25' below WT	79	57.7			
≥25' below WT	27	19.7			
≥50' below WT	13	9.5			
≥75' below WT	18	13.1			

* L=Log-normal distribution

** Total cases 137, missing cases 188

depends, in part, on the size of the ZOC. Since ZOC size is related to hydraulic conductivity, a value that is imprecisely known, we wanted to develop other measures of atrazine usage that were independent of ZOC size.

Area - Two variables describe area -- 1) the total area of the ZOC and 2) the total area of the fields where atrazine was applied. These variables were always treated as continuous variables.

Mean application rate - Application rates provide area-integrated measures of atrazine load that do not depend on the size of the ZOC. Mean application rate was calculated as:

$$\frac{\text{total load (lbs)/12 years}}{\text{area}}$$

We calculated a mean application rate averaged over the area of the fields that received atrazine and over the entire ZOC area. We felt that ZOC-area-averaged application rate would account for the fact that most ZOCs received atrazine over only a portion of their area. Water recharging in the areas not receiving atrazine could, conceivably, dilute the atrazine applied in other portions of the ZOC. The field-averaged atrazine application rate provides a higher estimate of atrazine use because it only considers those portions of the ZOC receiving atrazine.

Table 11. Descriptive statistics for land-use variables.

	Mean*	Median	Std dev	Minimum	Maximum	Distrib**
Total load (lbs)	216.3	139.2		1.1	2023.4	L
Category	*Frequency*	*Percent*				
.01 - 45	77	23.7				
46 - 135	83	25.5				
136 - 270	87	26.8				
> 270	78	24.0				
ZOC area (acre)	27.2	20.7		2.4	307.2	L
Field area (acre)	10.6	12.9		0.26	203.1	L
Mean annual application rate for ZOC (lbs/acre)	0.62	0.54		0.01	2.74	L
Category	*Frequency*	*Percent*				
< 0.3	81	24.9				
0.3 - 0.5	66	20.3				
0.5 - 0.8	91	28.0				
>0.8	87	26.8				
Mean annual application rate for fields (lbs/acre)	0.97	0.85	0.58	0.07	5.00	N
Category	*Frequency*	*Percent*				
<.6	69	21.2				
0.6 - 0.85	88	27.1				
0.85 - 1.0	58	17.8				
>1.0	110	33.8				

* Means are geometric for log-normal distributions, arithmetic for normal distributions

** L=Log-normal distribution, N=Normal

Atrazine Concentration

The well-water samples were collected as part of the Grade A Dairy Farm Well Water Quality Survey (LeMasters and Doyle, 1989), the Rural Well Survey (LeMasters, 1990), or the study conducted by Bradbury and McGrath (1992). Analysis technique varied with the different sampling programs and sampling frequency was not consistent. Most wells were sampled only once, however, some wells were sampled multiple times. Most samples collected as part of the Rural Well Survey were analyzed using the inexpensive immunoassay procedure which measures concentration of triazine-based compounds. The detection limit for this analysis method was 0.1 μg/l. Samples collected as part of Grade A Dairy Farm Survey or by Bradbury and McGrath were analyzed by the DATCP Bureau of Laboratory Services using the neutral extractable method developed by the State Lab of Hygiene (method

1200); results include measures of atrazine and metabolite concentrations. The detection limit for this method was 0.15 μg/l. As part of the Rural Well Survey, DATCP analyzed replicate samples in order to compare results from different analysis techniques. In general, the immunoassay technique provided reliable estimates of atrazine concentration except for samples with high atrazine concentrations; in these cases the method underestimated atrazine values (LeMasters 1990). Since the different analysis methods do not provide directly comparable measures of atrazine concentrations, we had to make judgements as to which values to use. For samples analyzed by the neutral extractable method we chose to use parent atrazine concentrations. For samples analyzed by the immunoassay procedure, we used the concentration of triazine-based compounds. If more than one analysis result was available for a given well (either total triazine concentration or parent atrazine concentration), because of multiple samplings or because of replicate analyses, we chose to use the highest value for our analysis. As a simplification we refer to all sampling results as "atrazine values" or "atrazine concentrations".

Given that the atrazine value for a given well may be based on a one-time sampling and that samples were collected under different methodologies and analyzed by different techniques, we were not confident in using the absolute value of atrazine concentration in our statistical analyses. Rather we used a flag indicating detect/no detect and generalized concentration categories based on approximate quartiles of the population (see Table 12).

Table 12. Descriptive statistics for atrazine variables*.

	Geometric Mean	Median	Minimum	Maximum	Distrib**
Atrazine concentration (μg/l)	0.325	0.11	0.00	4.80	L
Category	*Frequency*	*Percent*			
Below detection	156	48.0			
>0 - 0.2	39	12.0			
.2 - .2999	51	15.7			
.3 - .4999	30	9.2			
=>.5	49	15.1			
Atrazine detection					
No detect	156	48.0			
Detect	169	52.0			

* Results from immunoassay analysis technique are concentrations of triazine-based compounds whereas results from neutral extractable technique are atrazine concentrations. Geometric mean calculated for wells with detections; median determined using all results with non-detection = 0.0

** L=Log-normal distribution

Wells Excluded from Analysis

Wells were excluded from analysis for the following reasons:
- possible point source of atrazine contamination (15),
- low confidence in ZOC determination (33),
- no atrazine applied to ZOC (42), or
- data errors (2).

Several of the excluded wells could be included in more than one of the above categories. For example, the ZOC confidence was coded as low for five wells receiving no atrazine. These wells appear in two of the above categories. The original data set contained 397 wells, excluding the above wells left 325 data points.

Wells were excluded as possible point sources based on a variety of information; some objective and some subjective. DATCP conducted site investigations of wells with high concentrations of atrazine and determined that three of the wells in our original population were probably contaminated by point sources or a combination of both point and non-point sources. Rob McGrath concluded that one of the wells he sampled had been contaminated by a point source. The Cottage Grove Co-op is the site of a known atrazine spill. Several wells located within 1/4 to 1/2 mile of the site exhibited atrazine concentrations that were higher than other wells in the area and so we choose to exclude nine wells near the co-op. In addition, we excluded two wells based on a subjective evaluation of concentration in relation to load and physical characteristics. These wells exhibited unusually high atrazine concentrations (1.8 and 8.4 $\mu g/l$) in relation to the physical and land-use characteristics of the ZOC.

After evaluating confidence in ZOC determination (described earlier in this chapter) we chose to exclude 33 wells where our confidence in the ZOC was low. Data errors lead to the deletion of two wells, for one we had no concentration data and for another we had no land-use or soils data.

After completing our determination of land use and estimation of atrazine usage there were 42 ZOCs that had received no atrazine load; 27 had no atrazine detection and 15 had detections. We hoped that examination of the anomalous wells (detections but no atrazine load) would help identify weak points of our analysis. We determined that the delineation of ZOC boundaries was responsible for most of the anomalies.

Analysis Methods

The primary goal of this study was to determine which soils, geologic, and hydrogeologic factors are important in controlling the distribution of atrazine detections in domestic wells. We used a variety of statistical tools to look for correlations between these factors and atrazine detections. Qualitative indicators of correlation between two or three variables include scatter plots, three-dimensional scatter plots, and cross-tabulation tables comparing two variables. Quantitative measures of correlation include calculation of correlation coefficients. Multivariate techniques include cluster analysis, discriminant analysis, and logistic regression method.

Bivariate and Trivariate Techniques

Determining relationships between each independent variable and the dependent variable (in this case atrazine concentration) is a necessary step in any statistical analysis that involves numerous independent variables.

Scatter plots - Most of the continuous variables listed in Tables 7 to 12 are best described by a log-normal or normal distribution. For each of these variables we developed two-dimensional scatter plots of the nominal values (for normal distributions) or the log-transformed values versus the log-transformed atrazine concentrations. By using different symbols to indicate one of the categorical variables, we could use the two-dimensional scatter plots to examine the relationships between a continuous variable, a discrete variable, and atrazine concentration. The three-dimensional scatter plots generally included the log-transformed atrazine load values as the second independent continuous variable.

Scatter plots provide qualitative information concerning trends in the data, however, they provide no measure of the strength of the trend. Correlation coefficients are the standard measure of the strength of a linear relationship between two variables. Calculation of correlation coefficients assumes that the populations being compared are normally distributed and that their variances are similar. The log-transformation of much of our data allows us to meet the first assumption, however, Tables 7 to 12 indicate that the continuous variables have a wide range of variances. The log transformation mitigates this to some degree, but not enough to allow the calculation of any of the parametric measures of correlation.

Cross-tabulation - Cross-tabulation tables provide a way to compare two categorical variables. We developed cross-tabulation tables for many of the discrete variables listed in Tables 7 to 12; most of the tables were controlled by a secondary variable. For example if we wanted to look at both silt thickness and application rate we would first calculate a table that determined the percent detections of atrazine for differing silt thickness categories. In controlling the cross-tabulation by atrazine rate, we would then calculate successive tables for the different application rate categories so we could determine if the percent detections in any of the silt thickness classes changed as application rate increased.

Cross-tabulation tables may suggest that the populations being compared are statistically different. We used the non-parametric Pearson chi-square statistic (Norušis, 1992; SPSS Base System User's Guide, p 199-200) to test the null hypothesis that the two variables being compared were independent. The test compares the number of expected values for each cell if the variables were independent to actual number of values in each cell. Once the expected and actual counts have been determined, the test statistic is calculated and compared to the theoretical chi-squared distribution to estimate how probable the value is if the variables are independent. At small observed significance levels, the null hypothesis is rejected, and we conclude that the variables are related in some way.

In some cases, the variables used in the cross-tabulation table were categorized from a continuous variable. For example, the categories of detection and non-detection were derived from the atrazine concentration data. If the cross-tabulation suggested that there was a different percentage of atrazine detections between two categories (for example wells with and without shale within the ZOC) we used the continuous data to look for differences in geometric means between the two populations.

Multivariate Techniques

Multivariate statistical techniques explore the relationships between many independent variables and one dependent variable. Multiple linear regression techniques are probably the most well-known of multivariate techniques, however, these techniques require that the populations used in the analysis have similar variances. Our data cannot meet this assumption and so we used some non-parametric multivariate tools.

Classification - Both discriminant analysis and hierarchical cluster analysis are statistical techniques that attempt to classify objects or cases into similar categories by grouping together similar variables. Discriminant analysis requires 1) that membership is known for the cases used to describe the classification rule, 2) that the variances of the independent variables be similar, and 3) that the variables be continuous rather than categorical. Hierarchical cluster analysis makes no assumptions about variance, type of data, or about membership. At the beginning of the analysis, membership for all cases is unknown and even the number of groups is unknown. This technique can be used to cluster cases or variables; we used it to examine relationships between variables.

Logistic regression - Unlike multiple linear regression, logistic regression is a non-parametric multivariate statistical method that requires no assumptions concerning population distributions or variances and can use categorical as well as continuous independent variables (Norušis, 1992). Logistic regression can be used as a screening tool to identify the most important variables for prediction of certain events (for example atrazine detection). These variables can then be used to develop predictive models.

A general logistic regression equation is

$$Prob(event) = \frac{1}{1 + e^{-(B_0 + B_1 X)}}$$

where X is the independent variable, B_0 is the intercept, and B_1 is a slope coefficient for the independent variable (Norušis, 1992). For p independent variables, the model can be written

$$Prob(event) = \frac{1}{1+e^{-z}}$$

where Z is the linear combination

$$Z = B_0 + B_1 X_1 + B_2 X_2 + \ldots + B_p X_p \, .$$

The logistic regression method has been used to predict nitrate concentrations in surface water from land-use and hydrologic data (Mueller and others, 1993). We used logistic regression as a screening tool to identify significant variables and then used those land-use, soils, and hydrogeologic variables to develop predictive models. The goal of these models is to predict two events; the detection of atrazine and the presence of atrazine concentrations above the PAL of 0.3 μg/l. We developed predictive models for each of these events using three groupings of wells -- 1) all 325 wells, 2) wells in the glaciated area, and 3) wells in the unglaciated area. We assumed that different hydrogeologic processes might be important in glaciated and unglaciated areas. Comparison of the predictive accuracies of the models developed for different areas was used to test this assumption. The final groupings resulted in six predictive models.

For each of the six models, we used an iterative process to enter variables into the regression equation one at a time. Independent variables were incorporated into the models in order of the magnitude of the significance level of their slope coefficient (score statistic), using a process of forward stepwise selection. Slope coefficients were fit to the dependent variable through a method of maximum-likelihood which selected coefficients to optimize predictive accuracy of the model. Variables were added to the model if the score statistic was less than 0.15, and were removed from the model if their score statistic increased to greater than 0.20.

In order to check for cross-correlation among the independent variables, an initial model was developed to predict detection/non-detection for all 325 wells. In general, continuous variables were available for selection. We determined the strength of correlation for each independent variable relative to atrazine detection. For groups of cross-correlated variables, these were compared and the most strongly correlated variable was retained. Results of this cross-correlation analysis were assumed to apply for all subsequent models.

For each of the six models, initial analyses were run that used both the continuous and categorical data for each variable. We used non-transformed continuous variables. Models were re-run after selecting either the continuous or discrete data for a given variable, whichever showed the stronger correlation to the dependent variable.

Results

The relationships between atrazine detections and the variables describing soils, geologic, hydrogeologic, and land-use factors were difficult to quantify. Of the bivariate and trivariate techniques used, cross-tabulation of categorical data proved most useful. Attempts to use the continuous data to quantify the general trends suggested by the categorical cross-tabulation tables were generally unsuccessful. For example, the cross-tabulation of atrazine application rate versus atrazine detection (Table 13) suggests that there are higher percentages of detections at higher rates. The log-log scatter plot of mean annual atrazine application rate (over entire ZOC) versus atrazine concentration indicates that there is not a strong linear relationship between these two variables (see Figure 9). Many of the continuous variables have large variances, this tends to obscure the weak trends seen in the categorical data.

Logistic regression proved to be the most useful of the multivariate techniques. Cluster analysis of variables tended to confirm our ideas of which variables were most similar without providing any new insights. Variables combined into similar clusters approximately matched the soils, geologic, hydrogeologic, and land-use categories that we had previously defined.

Table 13. Cross-tabulation table of ZOC-averaged atrazine application rates and atrazine detections.

Application Rate *(lbs/acre)*	**Frequency** *Detect*	*No Detect*	**% Detections**
< 0.3	39	42	48.1
.3 - 0.5	30	36	45.5
0.5 - 0.8	47	44	51.6
>0.8	53	34	60.9

Three of the statistical analysis methods -- spatial exploration of the data, cross-tabulation, and logistic regression helped identify factors that seemed of primary importance in predicting whether a given domestic well would contain atrazine. We first present the details of the model developed to predict atrazine detections for all wells, a general discussion of the other five models, and a comparison of their predictive accuracy. This is followed by a detailed discussion of both primary and secondary variables.

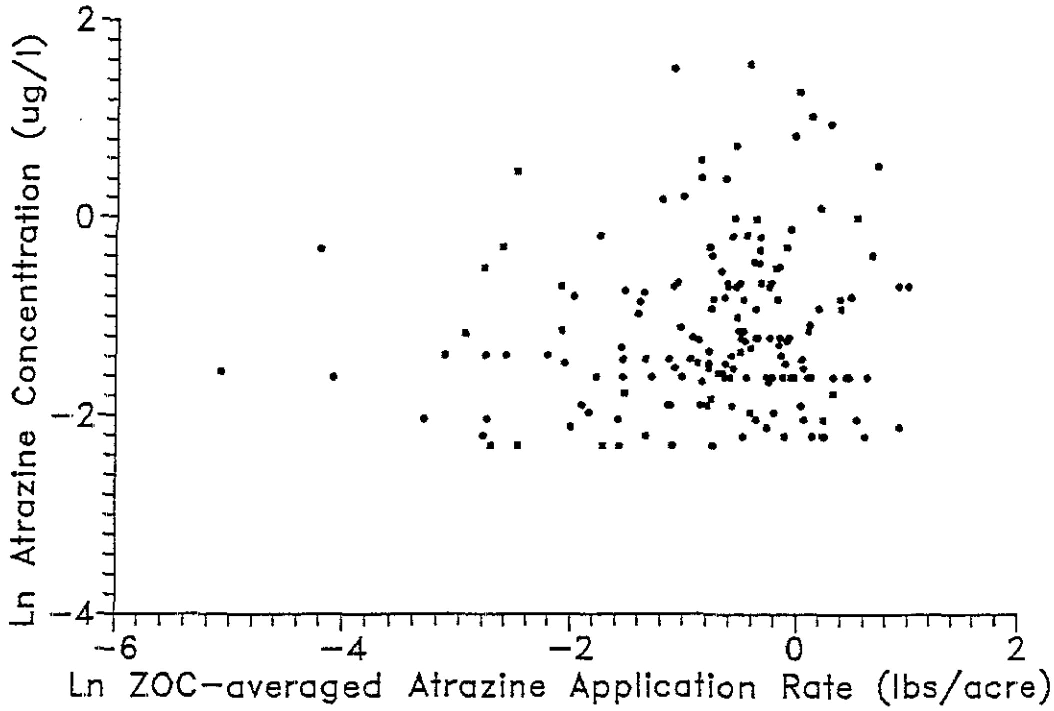


Figure 9. Scatter plot of log-transformed ZOC-averaged atrazine application rates versus log-transformed atrazine concentrations.

Predictive Models

Logistic regression uses a set of independent variables to estimate the probability of an event occurring. We used the method as a screening tool to identify which variables are important for prediction of atrazine detections and atrazine concentrations above the PAL. We developed predictive models for both atrazine detection and PAL exceedence using 1) all wells, 2) wells in the glaciated area, and 3) wells in the unglaciated area. The model for prediction of atrazine detection developed with data from all wells is used to identify the relative importance of the independent variables.

The logistic regression statistic (R) allows us to assess the contribution of individual variables to a model. R values range from -1 to +1 and are a measure of the partial correlation between the dependent variable and each independent variable; positive values indicate positive correlation. The absolute value of R indicates the strength of the contribution to the model; smaller absolute values indicating less contribution. Significance values indicate the confidence in the variable as a predictor. For example, a significance value of .05 indicates a 95% confidence level.

Table 14 summarizes the logistic regression model for the prediction of atrazine detections using data from all wells. The table lists independent variables in order of decreasing importance as well as the associated slope coefficient, R statistic, and statistical significance level. The R values indicate that the variables with the largest contributions to the predictive equation are the presence of *Sinnipee Group dolomites* (-0.1756), presence of shale or clay (-0.1463), total atrazine load (0.1202), thickness of saturated unlithified materials (-0.0990), and location in discharge area (-0.0863). With the exception of the unlithified vadose thickness and two of the silt thickness categories, variables in the predictive equation in Table 14 are significant at a 95% confidence level.

Table 14. Logistic regression model for prediction of atrazine detection developed using data from all wells.

Independent Variable	Slope Coef	R Statistic	Signif.
Sinnipee Group	-1.6885	-.1756	.0001
Shale/clay	-.9707	-.1463	.0007
Total atrazine load	.0017	.1202	.0036
Thickness of saturated unlithified material	-.0360	-.0990	.0113
Discharge area	-.7852	-.0863	.0207
Soil thickness	-.0255	-.0785	.0289
Bedrock depth	.0270	.0676	.0441
Unlithified vadose thickness	-.0213	-.0210	.1382
Silt thickness (category)		.0000	.1418
silt thickness(1)	.3148	.0142	.1482
silt thickness(2)	-.4845	-.0768	.0309
silt thickness(3)	.1148	.0000	.5925
Constant B_0	1.2378		.0084

Choice of variables and relative importance of the variables vary for each of the predictive models. Presentation of the details of each model is not particularly illustrative. However, comparison of models developed for glaciated and unglaciated areas indicate that other variables, in addition to those identified in Table 14, may be important in predicting atrazine occurrence. Results from all models, along with results from spatial exploration and cross-tabulation were used to identify both primary and secondary variables. The predictive capabilities of the models are outlined below followed by a description of primary and secondary variables.

<u>Comparison of predictive models</u> The models can be evaluated for predictive accuracy through comparison of predicted and observed results. Table 15 compares the observed

atrazine detections and PAL exceedences to those predicted by each of the models. Results are compared for models developed with all wells, wells in glaciated areas, and wells in unglaciated areas. The overall predictive accuracy (percent correct predictions) and bias of each model has been evaluated. Models can be biased in terms of the predictive accuracy for

Table 15. Comparison of observed atrazine detections and PAL exceedences with logistic regression model predictions.

			Predicted Classification			
Model	**Category**	**Observed**	*frequency*	*%*	*frequency*	*%*
ALL WELLS			**Correct**		**Incorrect**	
Detection	No Detect	156	97	62	59	38
	Detect	169	116	69	53	31
		325	*Overall %*	*66*	*Overall %*	*34*
PAL Exceedence	< PAL	246	235	96	11	4
	≥ PAL	79	13	16	66	84
		325	*Overall %*	*76*	*Overall %*	*24*
GLACIATED			**Correct**		**Incorrect**	
Detection	No Detect	89	57	64	32	36
	Detect	115	91	79	24	21
		204	*Overall %*	*73*	*Overall %*	*27*
PAL Exceedence	< PAL	150	145	97	5	3
	≥ PAL	54	9	17	45	83
		204	*Overall %*	*75*	*Overall %*	*25*
UNGLACIATED			**Correct**		**Incorrect**	
Detection	No Detect	67	53	79	14	21
	Detect	54	28	52	26	48
		121	*Overall %*	*67*	*Overall %*	*33*
PAL Exceedence	< PAL	96	89	93	7	7
	≥ PAL	25	13	52	12	48
		121	*Overall %*	*84*	*Overall %*	*16*

different categories of the dependent variable (*i.e.* detection/non-detection or exceedence/non-exceedence), for different geographic areas, or for different subsets of wells. We examined the model bias in terms of the predictive accuracy of different categories of the dependent variable.

All six models show reasonable overall predictive success, ranging from 66% to 84% correct classification. Most of the models show some bias, however, which can limit their usefulness. The model for prediction of atrazine detections for all wells is a relatively unbiased predictor of the dependent variable, with 62% of non-detections and 69% of detections correctly classified.

The models developed to predict atrazine concentrations exceeding the PAL generally had good overall predictive accuracy, however, the predictive capability was strongly biased and these models were poor predictors of PAL exceedences. For all wells, the PAL exceedence model has an overall prediction rate of 76%, however, only 16% of the exceedences are correctly classified. The model developed for the Driftless Area shows better predictive success, but is still a poor predictor of concentrations above the PAL.

Models developed for subsets of the data-- wells located in the glaciated and unglaciated areas-- show improved accuracy for prediction of atrazine detections compared to the model that used all wells. The models, however, are biased; the model for the glaciated area is a better predictor of detections and the model for the unglaciated area is a better predictor of non-detections. The improved overall accuracy of the stratified models is probably due to the fact that stratification allows different variables to be selected for the different geographic regions. The glaciation variable is not chosen in the models developed for all wells because there are no strong trends in either percent detection or PAL exceedence with glaciation.

Primary Variables

Spatial exploration of the data, cross-tabulation results, and logistic regression helped identify variables that seemed of primary importance in predicting atrazine detections or PAL exceedences. These factors include atrazine use, presence of clay or shale, presence of Sinnipee Group dolomite as the uppermost bedrock unit over the majority of the ZOC, and location in a discharge area. We discuss each of these factors in the following section and present results from both cross-tabulations and logistic regression analyses.

<u>Atrazine use</u> - Spatial exploration of the data, cross-tabulation (Table 13 and Figure 9), and logistic regression (Table 14) all indicate a positive trend between increasing atrazine usage and atrazine detections. Cross-tabulation suggests a weak positive trend between ZOC-averaged atrazine application rate and percent detections. The logistic regression procedure indicates that total atrazine load is strongly correlated with atrazine detections. Total atrazine load, listed third in Table 14, is one of the most important variables for predicting atrazine detections for all wells.

Presence of shale or clay - There are 85 ZOCs that contain appreciable shale or clay sequences (see p. 32) and both cross-tabulation and logistic regression identify this as an important variable. Table 16 summarizes the cross-tabulation of presence of shale/clay versus percent detections. The entire dataset (all 325 wells) has a 48% non-detection rate; wells with shale have a non-detection rate of 61% (39% detection). The Pearson chi-square statistic indicates that the variables are not independent (at the 95% confidence limit). To further compare these two subsets, we determined both the median atrazine concentration using data from both detections and non-detections (coded as 0.0) and the geometric mean concentration for wells with detections. Wells with shale have a geometric mean concentration of 0.234 μg/l (median 0.0 μg/l) whereas wells without shale have a geometric mean concentration of 0.351 μg/l (median 0.135 μg/l). These differences in median concentration, geometric mean concentration, and percent detections all suggest that the presence of shale or clay within the ZOC tends to attenuate atrazine. In addition, the general logistic regression model (Table 14) indicates that this variable is the second most important variable in terms of predicting atrazine detections for all wells.

Table 16. Cross-tabulation table of presence of shale or clay and atrazine detections.

Presence of shale/clay	**Frequency** *Detect*	*No Detect*	**% Detections**	**Geometric Mean** *$\mu g/l$*	**Median** *$\mu g/l$*
Present	33	52	39.0	0.234	0.0
Absent	136	104	57.0	0.351	0.135

Presence of Sinnipee Group dolomite as uppermost bedrock unit - The Sinnipee Group dolomite is the uppermost bedrock unit over the majority of 49 ZOCs in the unglaciated area (see p. 32 and Figure 8). The cross-tabulation table (Table 17) indicates that the percent detection for these 49 wells is much less than the entire dataset. The Pearson chi-square statistic confirms that the variables are not independent. Both median concentrations (all wells) and geometric mean concentrations (wells with detections) are lower for ZOCs where the Sinnipee Group dolomite is the uppermost bedrock unit. Logistic regression also identifies this as an important predictor of atrazine detection for all wells (see Table 14).

There are many possible geologic reasons why the area with Sinnipee dolomite as the uppermost bedrock unit seems to attenuate atrazine. The Sinnipee Group overlies the St. Peter sandstone and is composed of the Platteville, Decorah, and Galena Formations. The Sinnipee occurs high in the landscape and is not commonly saturated. Wells in this area are completed in the underlying St. Peter or Prairie du Chien Formations. The St. Peter unconformably overlies the Prairie du Chien dolomite and the base of the unit is sometimes shaley. The "red ochre" noted in some WCRs is probably weathered Prairie du Chien dolomite and it tends to be fine-grained. The fine-grained base of the St.Peter might provide

Table 17. Cross-tabulation table of presence of Sinnipee Group dolomite as the uppermost bedrock unit and atrazine detections.

Presence of Sinnipee	Frequency *Detect*	*No Detect*	% Detections	Geometric Mean $\mu g/l$	Median $\mu g/l$
Present	15	34	30.6	0.273	0.0
Absent	154	122	55.8	0.330	0.125

attenuation for wells completed below this. Shales and bentonite (clay) layers within the Platteville and Decorah Formations might also provide attenuation, especially for wells completed above the base of the St. Peter.

The Sinnipee is in the upper portion of the stratigraphic sequence in Dane County. Ostrom (1965) noted a generally fining-upward trend for this sequence. The Cambrian period is characterized by deposition of relatively clean sandstones; carbonates become dominant in Ordovician time and both the Prairie du Chien and Sinnipee dolomites are deposited during this period. There seem to be differences in attenuation potential between the Ordovician dolomites. We determined the uppermost formation for all sampled wells (at the location of the well) and determined percentage atrazine detections for different units. If we compare wells in the Driftless Area, the Prairie du Chien dolomite had 56.3% detections (9 of 16) while the Sinnipee had 30.6% detections (15 of 39). This is not a totally equivalent comparison because the presence of Sinnipee was determined for the entire ZOC area rather than at the point location of the well, however, it suggests that the younger Sinnipee dolomite is better able to attenuate contaminants than the Prairie du Chien dolomite.

Roundtree Formation: The Roundtree Formation, as described by Clayton and Attig (1990) consists of a relatively continuous sheet of clay that occurs on the Oneota uplands in western Sauk County and on Prairie du Chien and Sinnipee uplands elsewhere in the Driftless Area. Several soil series, specifically the Ashdale, Dodgeville, Dunbarton, Edmund, and New Glarus, are developed in chert-rich clay. We assumed that this clay is equivalent to the Roundtree Formation and we have used the soils information to generate maps showing the approximate extent of the Roundtree Formation in Dane County. The generalized area where the Sinnipee is the uppermost bedrock unit (Figure 8) also included the majority of the area where the Roundtree Formation was present. The presence of the Roundtree Formation is another possible attenuation factor in this area.

<u>Location in discharge area</u> - The logistic regression model developed with data from all 325 wells indicates that location in a discharge area is an important variable for prediction of atrazine detection. Spatial exploration of the data suggested that discharge wells, excluding those in the Wisconsin River Valley, exhibited lower overall atrazine concentrations than wells located in recharge areas or in the middle of the flow system. We calculated percent

detections and geometric mean atrazine concentrations for recharge, middle, and discharge wells. Geometric means were calculated using wells with atrazine detections. We categorized ZOC-averaged annual atrazine application rate as < 0.5 lbs/acre or > 0.5 lbs/acre (see Table 18). Further categorization resulted in subsets with too few values (< 5) to calculate geometric mean atrazine concentrations

Table 18. Cross-tabulation of position in flow system and geometric mean atrazine concentrations categorized by ZOC-averaged atrazine application rate (excluding WI River Valley wells).

Mean Annual Applic. Rate *(lbs/acre)*	**Flow System Position**	**Geometric Mean Atrazine** *(μg/l)*	**Frequency** *Detect*	*No Detect*	**% Detections**
< 0.5	R	0.349	13	13	50.0
	M	0.286	47	42	52.8
	D	0.213	9	21	30.0
> 0.5	R	0.344	16	15	51.6
	M	0.347	59	48	55.1
	D	0.307	16	13	55.2

At ZOC-averaged annual application rates < 0.5 lbs/acre, wells located in discharge areas had 30% detections compared to 50% for wells in recharge areas and 52.8% for wells in the middle of flow systems. At application rates > 0.5 lbs/acre, wells in all parts of the flow system had more than 50% detections. Comparing the geometric mean atrazine concentrations for the three categories of wells at application rates < 0.5 lbs/acre, suggests that concentrations are highest in recharge areas, decreasing in the middle portions of flow systems and in discharge areas. This trend is not seen at higher application rates.

Recharge ares are characterized by predominantly downward groundwater flow and young, recently recharged groundwater. Atrazine concentrations in wells in these areas is strongly influenced by land-use activities immediately adjacent to the well. By contrast, discharge areas are characterized by upward flow. Some of the water reaching these discharge areas travels along deep, more regional flow paths. This water tends to be older and is less likely to be contaminated by agricultural chemicals. Wells located in discharge areas may receive some of their water from the delineated ZOC and some water from regional flow paths. The effect of the regional flow paths may be to dilute any atrazine recharged from the delineated ZOC. Wells in the Wisconsin River Valley are an exception to this trend. Of the 13 wells in the valley, all are classified as discharge and 9 (or 69.2%) have detections. In Dane County, the Wisconsin River Valley is an area of intensive irrigated agriculture. Atrazine loads are high, the water table is shallow, soils have limited attenuation potential (Lowery and McSweeney, 1992), and the wells are completed in coarse sand and gravel. Irrigation helps draw atrazine from the water table to deeper in the saturated zone. The combination of these physical and land-use factors apparently overrides any dilution by regional flow systems.

Secondary Variables

Variables of secondary importance in predicting atrazine detections were identified by cross-tabulation and by logistic regression. Each of the six logistic regression models ranked the explanatory variables in terms of relative importance to the predictive equation. These rankings were used in combination with cross-tabulation tables to identify secondary variables. In order to use cross-tabulation to explore secondary trends we needed to stratify the dataset by attenuating variables. Location in discharge area, presence of shale within the ZOC, or presence of Sinnipee Group dolomite as the uppermost bedrock unit over the majority of the ZOC are identified as primary variables that tend to attenuate atrazine. We identified few trends between other soils, geologic, hydrogeologic, or well-construction variables and atrazine detections unless we also stratified on the attenuating variables. For example, when we examined the soils variables (soil thickness, SCAM2 ranking, and silt thickness), the trends were easier to identify if we examined just non-attenuated wells. Once we identified potential trends we examined the entire dataset to determine if these trends were robust. The following section, "Secondary Variables", summarizes the trends we noted for the soils, geologic, hydrogeologic, and well-construction variables.

<u>Soils</u> - We examined soil thickness, SCAM2 ranking, and silt thickness. Some of these variables included trends that were counter-intuitive.

Soil thickness, at the point location of the well, was identified as an explanatory variable for prediction of atrazine detections by the logistic regression analysis of all wells (see Table 14). The negative slope coefficient indicates that detections are less likely with deeper soils. Cross-tabulation did not identify a clear trend between soil thickness and atrazine detections. Wells with soils <6 inches or >30 inches have detection rates less than the overall detection rate of 52% (see Table 19). The low detection rate for wells with very shallow soils may be due to the presence of the Roundtree Formation. This fine-grained surficial unit is present on uplands in the Driftless Area and may be one of the geologic factors that attenuate atrazine in the area where Sinnipee dolomite is the uppermost bedrock unit (see discussion above).

Logistic regression identified area-averaged SCAM2 ranking as an important predictor of PAL exceedence for all wells. Cross-tabulation also suggests trends when the area-averaged SCAM2 rankings are categorized by ZOC-averaged atrazine application rate (Table 20). Zones of contribution with SCAM2 rankings falling in the "least" attenuation category always show more detections than non-detections, regardless of atrazine rate. Area-averaged "marginal" and "good" rankings show fewer detections at lower rates, but this does not hold at higher rates. These results were expected, however, "best" rankings show more detections

Table 19. Cross-tabulation table of soil thickness categories and atrazine detections.

Soil Thickness *(in)*	Frequency *Detect*	*No Detect*	% Detections
≤ 6	17	26	39.5
7-18	29	22	56.9
19-30	85	54	61.2
31-42	31	44	41.3
>54	7	10	41.2

than non-detections for 3 out of 4 application rate categories. This may not indicate a failure in the "best" classification. These "best" soils have been farmed intensively for a long period of time. Our rate category, determined from a 12-year cropping history, may underestimate the amount of atrazine applied to these soils.

Table 20. Cross-tabulation of area-weighted SCAM2 rankings and atrazine detections categorized by ZOC-averaged atrazine application rate.

Mean Annual Application *(lbs/acre)*	**SCAM2 Ranking**	**Frequency** *Detect*	*No Detect*	**% Detections**
< 0.3	least	4	3	57.1
	marginal	8	13	38.0
	good	17	22	43.6
	best	10	4	71.4
0.3 - 0.5	least	5	4	55.6
	marginal	6	14	30.0
	good	13	16	44.8
	best	6	2	75.0
0.5 - 0.8	least	5	2	71.4
	marginal	11	16	40.7
	good	24	18	57.1
	best	7	8	46.7
> 0.8	least	6	3	66.7
	marginal	10	5	66.7
	good	21	18	53.8
	best	16	8	66.7

Silt thickness also exhibits an unexpected trend, categories of greater silt thickness show more detections than categories of less silt thickness (see Table 21). We tried to examine silt thickness in relation to atrazine application rates, however, we ended up with too few values (< 5) to calculate meaningful percent detections.

Table 21. Cross-tabulation table of area-weighted silt thickness categories and atrazine detections.

Area-weighted Silt Thickness *(in)*	**Frequency** *Detect*	*No Detect*	**% Detections**
0 - 13.9	30	34	46.9
14 - 21.2	31	32	49.2
21.3 - 27.3	35	29	54.7
> 27.4	39	23	62.9

Geologic - We examined several geologic variables including depth to bedrock, type and texture of unlithified materials, and uppermost bedrock unit. Logistic regression identified depth to bedrock, as determined at the well, as an important predictor of atrazine detection. Table 22 summarizes the depth-to-bedrock data. The wells in the 0-5 ft category have only 34.7% detections while all other depth-to-bedrock categories indicate over 49% detections. The low detection rate for shallow bedrock wells may be due to location in the area with Sinnipee dolomite (59% of these wells are located in this area) or presence of the Roundtree Formation in the ZOC (80% of these wells also have Roundtree in the ZOC). Comparison of atrazine application rates for the different depth-to-bedrock categories did not indicate that areas with shallow bedrock received any less atrazine than other areas.

Table 22. Cross-tabulation table of depth-to-bedrock categories and atrazine detections.

Depth to bedrock *(ft)*	**Frequency** *Detect*	*No Detect*	**% Detections**
0-5	17	32	34.7
6-10	22	15	59.5
11-50	53	47	53.0
51-100	53	37	58.9
>100	24	25	49.0

The type of unlithified material showed weak trends in relation to atrazine detections. Coarse-grained unlithified materials (see p. 30 and Table 8 for description of categories) had more detections (56.3%) than fine-grained unlithified materials (41.7% detections). Further categorization did not yield any identifiable trends. In addition, the unlithified categories for weathered bedrock generally showed fewer detections (weathered dolomite 18 of 43 or 41.9% detections, weathered sandstone 10 of 26 or 38.5% detections, weathered shaley sandstone 3/6 or 50% detections).

Based on Bradbury and McGrath's (1992) work, we expected to see a trend in detection rate based on the uppermost bedrock type (see p. 30 and Table 8 for description of categories). Logistic regression identified uppermost bedrock depositional environment code as the most important predictor of atrazine detections and PAL exceedences in the Driftless area. Cross-tabulation suggests that dolomite bedrock has a higher detection rate than the other bedrock depositional environments (see Table 23). This trend may be complicated by differences in the dolomite. As noted above, the Sinnipee tends to have a lower detection rate than the Prairie du Chien. Wells completed in sand and gravel have the highest detection rate.

Hydrogeologic - Logistic regression identifies both thickness of unlithified materials in both the vadose and saturated zones as important variables for predicting atrazine detections. Both variables have negative slope coefficients which indicate that atrazine detections are less likely with increasing thickness of either unlithified vadose zone or unlithified saturated zone. Using cross-tabulation we were unable to identify robust trends between these variables and atrazine detection.

Table 23. Cross-tabulation table of uppermost bedrock type and atrazine detections.

Type of bedrock/ Environment of Deposition Code	**Frequency** *Detect*	*No Detect*	**% Detections**
1. Clean Sandstone	54	64	45.8
3. Shaley Sandstone	15	18	45.5
4. Carbonate	82	68	54.7
5. Sand and Gravel	18	6	75.0

Well Construction - Our data set was limited to the 137 wells for which we had constructor's reports. Cross-tabulation suggests weak trends for casing depth below water table and well depth. The majority of wells were cased <50 ft into the water table (106); 49 of these wells (46.2%) had atrazine detections. Thirty-one wells were cased ≥50 ft into the water table, only 10 of these (32.2%) had atrazine detections. If we further stratify by glaciation, there is a weak trend suggesting that deeper wells have less detections, however, this trend is not evident in the non-glaciated area. We also explored the relationship between depth of casing below the water table to percent detections in discharge areas. There are 25 wells in discharge areas for which we have matching WCRs. Eight of these have casing <25 ft below the water table and only one (12.5%) had an atrazine detection. Seventeen have casing >25 ft below the water table and eight (47%) have detections.

Chapter VI.

CONCLUSIONS

Compilation of Land-use and Hydrogeologic Information

1. Geo-relational database methods, in which data tables were related through unique identifiers to geographic features in an ARC/INFO coverage, minimized the tabular data physically stored in the coverages. Analysis and display relied on dynamic joins to external data tables and lookup tables. One advantage of this approach is an easier update procedure for attributes -- corrections can be made to one file instead of multiple files.

2. Compiling domestic well-construction report information in a relational database and integrating the database with a geographic information system allow this information to be applied to a variety of problems. The well-construction report database contains data that can be used to construct water-table and depth-to-bedrock maps, calculate hydraulic conductivities, and estimate aquifer thickness and porosity.

3. PRETRAC, a pcARCPLOT application developed for this project, provides an interface between the relational database containing well-construction report data, the digital water-table map, and the TGUESS program to calculate hydraulic conductivity.

4. PRETRAC was used to develop input files for the GPTRAC model used to determine ZOC boundaries. The interactive capabilities of this application greatly simplified this task and reduced work volume.

5. PRETRAC's ability to display the modeled ZOCs with land-use as well as soils, geologic, and hydrogeologic characteristics provided a powerful and flexible data exploration tool.

6. PC ARC/INFO applications developed jointly by the Dane County Land Conservation Department and the UW Land Information and Computer Graphics Facility helped visually integrate land-use photos with farm field boundaries and the delineated ZOC boundaries. These interfaces greatly assisted the interpretation and compilation of crop histories.

Statistical Analysis

1. The diversity of hydrogeologic settings in Dane County was one reason we selected the county as the study area; this diversity greatly complicated our statistical analysis.

2. The relationships between atrazine detections and the variables describing physical and

land-use factors were difficult to identify and quantify. Non-parametric techniques such as cross-tabulation of categorical data and logistic regression for multivariate analysis proved to be the most useful. The wide range of variances for the continuous variables obscured weak trends seen in the categorical data.

3. Variables of primary importance in predicting whether a given domestic well would have an atrazine detection include 1) atrazine use, 2) presence of shale, 3) presence of Sinnipee Group dolomite as the uppermost bedrock unit over the majority of the ZOC, and 4) location in discharge area.

4. Logistic regression was used to incorporate both primary and secondary variables into predictive models. Models were developed for both atrazine detection and exceedence of PAL using all wells, wells in the glaciated area, and wells in the unglaciated area. The atrazine detection model developed using data from all wells had an overall predictive accuracy of 66% and was relatively unbiased with 69% of the detections accurately identified and 62% of the non-detections accurately identified. Models to predict PAL exceedences tended to have good overall predicative accuracy but were highly biased and poor predictors of PAL exceedences.

5. Soil thickness, unlithified materials, and depth-to-bedrock data all suggest that thin, fine-grained soils may be attenuating atrazine. This may be due to the presence of the fine-grained Roundtree Formation. The effect of this unit could not be examined directly because the majority of ZOCs containing the Roundtree Formation are located in the area with Sinnipee dolomite as the uppermost bedrock unit. There are geologic reasons that suggest the Sinnipee Group dolomite may also attenuate atrazine.

Implications and Recommendations

The relationships between atrazine detections and the variables describing soils, geologic, hydrogeologic, and land-use factors were difficult to identify and quantify. This study identifies land-use and the following factors as important predictors of atrazine detection for domestic wells in Dane County:

1) presence of shale or clay,
2) presence of Sinnipee Group dolomites,
3) location in discharge area.

Characterizing soils, geology and understanding the groundwater flow system are important for prediction of atrazine detections. Land-use and the geologic variables outlined above were determined for the land area that contributes water to the well (or zone of contribution, ZOC, of the well). Flow system position, especially location in a discharge area also appears to be important. Fine-grained units, either shale, clay layers in the Sinnipee, or thin fine-grained soils all appear to attenuate atrazine.

The statistical model developed to predict atrazine detection using the detailed soils, geologic, and hydrogeologic data for all 325 wells had overall predictive accuracy of 66%. Stratification of the data and development of separate models for the glaciated and unglaciated portions of the county led to improved overall predictive accuracy. This suggests that prediction of the distribution of atrazine detections is complicated by the variability of natural settings and that predictive models developed for smaller areas, with more consistent soils, geologic, and hydrogeologic characteristics are more likely to be accurate.

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