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ATRAZINE AND METOLACHLOR OCCURRENCE IN SHALLOW GROUND WATER OF THE UNITED STATES, 1993 TO 1995: RELATIONS TO EXPLANATORY FACTORS[1]

Dana W. Kolpin, Jack E. Barbash, and Robert J. Gilliom[2]

ABSTRACT: Since 1991, the U.S. Geological Survey has been conducting the National Water Quality Assessment (NAWQA) Program to determine the quality of the Nation's water resources. In an effort to obtain a better understanding of why pesticides are found in shallow ground water on a national scale, a set of factors likely to affect the fate and transport of two herbicides in the subsurface were examined. Atrazine and metolachlor were selected for this discussion because they were among the most frequently detected pesticides in ground water during the first phase of the NAWQA Program (1993 to 1995), and each was the most frequently detected compound in its chemical class (triazines and acetanilides, respectively). The factors that most strongly correlated with the frequencies of atrazine detection in shallow ground-water networks were those that provided either: (1) an indication of the potential susceptibility of ground water to atrazine contamination, or (2) an indication of relative ground-water age. The factors most closely related to the frequencies of metolachlor detection in ground water, however, were those that estimated or indicated the intensity of the agricultural use of metolachlor. This difference is probably the result of detailed use estimates for these compounds being available only for agricultural settings. While atrazine use is relatively extensive in nonagricultural settings, in addition to its widespread agricultural use, metolachlor is used almost exclusively for agricultural purposes. As a result, estimates of agricultural applications provide a less reliable indication of total chemical use for atrazine than for metolachlor. A multivariate analysis demonstrated that the factors of interest explained about 50 percent of the variance in atrazine and metolachlor detection frequencies among the NAWQA land-use studies examined. The inclusion of other factors related to pesticide fate and transport in ground water, or improvements in the quality and accuracy of the data employed for the factors examined, may help explain more of the remaining variance in the frequencies of atrazine and metolachlor detection.

(KEY TERMS: pesticides; ground water hydrology,; nonpoint source pollution; statistical analysis; water quality.)

INTRODUCTION

Numerous studies have examined the occurrence of pesticides in ground water of the United States over the past three decades (i.e., Hallberg, 1989; Holden *et al.,* 1992; Richards *et al.,* 1996; Springer and Bair, 1998). Although much of this research has focused on agricultural areas (Barbash and Resek, 1996), recent research has shown that urban use is also an important source of pesticide contamination in ground water (Bruce and McMahon, 1996; Bucheli *et al.,*1998; Capel *et al.,* 1999). Few studies, however, have been conducted at the national scale to provide information on both pesticide occurrence and an understanding of their fate and transport to ground water. In 1991, the U.S. Geological Survey began full-scale implementation of the National Water Quality Assessment (NAWQA) Program to examine the quality of the water resources of the United States (Leahy and Thompson, 1994; Gilliom *et al.,* 1995). The building blocks of this national assessment are water-quality studies in selected major watersheds (study units). The NAWQA study units are divided into three groups that are studied on a rotational schedule of three-year periods of intensive data collection. About one-third of the study units are in the intensive data-collection phase at any given time.

The results from the first phase of NAWQA (20 study units, sampled from 1993 to 1995) documented that pesticides are widely detected in ground water across the Nation (Gilliom *et al.,* 1999; Kolpin *et al.,* 2000). The pesticide concentrations encountered were

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generally low, with median total concentrations (summation of detected concentrations) being 0.046 µg/L (Kolpin *et al.,* 2000). Pesticides were commonly detected in shallow ground water beneath both agricultural and urban areas.

The purpose of this paper is to build upon the results presented in previous discussions of the pesticide data from the first phase of NAWQA (Kolpin *et al.,*1998; Barbash *et al.,* 1999; Gilliom *et al.,* 1999; U.S. Geological Survey, 1999; Kolpin *et al.,* 2000; Barbash *et al.,* 2001) to obtain a better understanding of the factors that may control their fate and transport to ground water on a national scale. The herbicides atrazine and metolachlor are used as examples in this statistical analysis of the data. These compounds were detected with a wide range of frequencies in ground water during the first phase of NAWQA, but have differing chemical and physical properties.

METHODS

Study Design

One focus of the ground-water component for NAWQA is through the design and sampling of "land-use studies." Land-use studies involve the sampling of either existing or newly installed wells to assess the quality of shallow (generally less than 30 m), recently recharged ground water in specific hydrogeologic settings dominated by specific types of land use. To ensure that water-quality data are comparable among the various land-use studies, consistent guidelines for study design and random site selection were used (Gilliom *et al.,* 1995; Lampham *et al.,* 1995; Scott, 1990). Pesticide data from 50 land-use studies during the first phase of the NAWQA program (1993 to 1995) were used for this analysis (Figure 1). Each land-use study was based on a one-time sampling of a set of sites selected at random from a targeted land use within a specific geographic area and hydrogeologic setting. Land-use studies that were comprised of fewer than ten sampling sites were excluded from this analysis. A summary of many of the principal features of these studies has been provided by Barbash *et al.* (1999), and is also available on the world-wide web at http://water.wr.usgs.gov/pnsp/fy91sum.html.

Sampling and Analytical Methods

All ground-water samples were collected using nationally consistent sampling protocols (Koterba *et al.,* 1995 or http://wwwrvares.er.usgs.gov/nawqa /OFR95-399.html) and analyzed for atrazine (reporting limit = 0.001 µg/L) and metolachlor (reporting

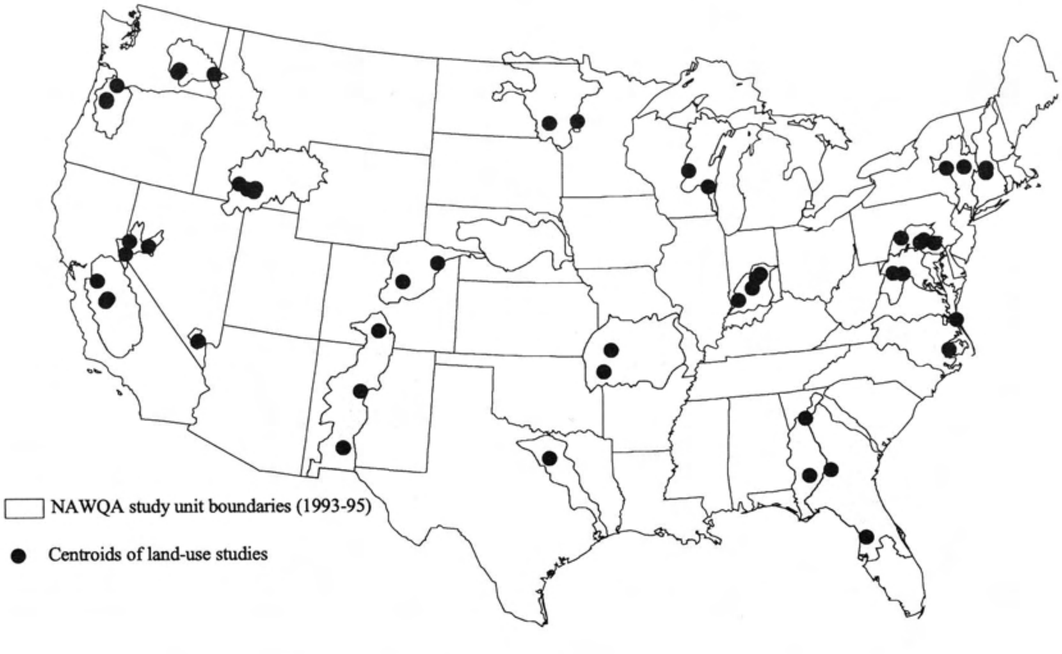

Figure 1. General location of the NAWQA Land-Use Studies, 1993 to 1995. The center of the land-use study being represented by the centroid.

limit = 0.002 µg/L) using gas chromatography/mass spectrometry (Zaugg *et al.,* 1995; http://water.wr.usgs.gov/pnsp/anstrat).

Ancillary Data

An attempt was made to obtain data for as many factors that affect the sources, transport, and fate of pesticides in ground water as possible. Table 1 lists the ancillary factors used for this statistical analysis. Most data were generated within a set circular distance (buffer) surrounding each of the sampled sites (Table 1). The procedure used to obtain the estimated agricultural use for atrazine and metolachlor are described elsewhere (Barbash *et al.,* 2001). The ancillary data were aggregated for each land-use study because the objective of this study was to understand the variability in pesticide detection frequencies among land-use studies, rather than the variability in pesticide concentrations among individual wells. Future work will examine factors controlling variations in pesticide concentrations among wells.

Statistical Analyses

Spearman rank correlation coefficients (Helsel and Hirsch, 1992; SAS, 1990) were calculated to examine the statistical significance of relations between the frequencies of pesticide detection (by land-use study) and all ancillary factors that were quantified by continuous variables. Spearman rank correlations provide a nonparametric measure of the monotonic relations between pairs of continuous variables. A significance level (α) of 0.05 was used for all of the statistical analyses. This acceptable probability of error ($\alpha = 0.05$) means that there is one chance in 20 that the statistical test reported a significant relation when one did not exist.

Parametric methods were also used to investigate statistical relations between the herbicide detection frequencies and the explanatory factors of interest (SAS, 1990). Multiple linear regressions were examined for both atrazine and metolachlor to identify the sets of ancillary factors that best predicted their respective frequencies of detection among the land-use studies from the first 20 NAWQA study units. All variables were log-transformed for this analysis (base 10) so that their statistical distributions would more closely approximate normality. To accommodate the log transformation, all zero values for a given factor were assigned a value less than the smallest nonzero value for that factor prior to transformation.

RESULTS

Although 67 different pesticide compounds were detected in ground water during the first phase of NAWQA (Kolpin *et al.,* 2000), the five that were most frequently detected accounted for the majority of the detections in the land-use studies (Figure 2). Statistical relations between explanatory variables (Table 1) and network detection frequencies are discussed here for two of these compounds, atrazine (the most frequently detected triazine herbicide) and metolachlor (the most frequently detected acetanilide herbicide).

Atrazine

The factors found to exhibit statistically significant Spearman rank correlations with the frequencies of atrazine detection ($P = 0.05$, Table 1) for the 50 land-use studies are shown in Figure 3, in order of increasing P (the probability that the relations arose by chance). Total nitrogen concentration (TN) showed the strongest such relation (Figure 3A). Because nitrogen fertilizers are commonly used in conjunction with pesticides to increase crop production, and because nitrate is frequently detected in aerobic ground water where such fertilizers are used (Nolan *et al.,* 1997; Nolan, 1999), TN may provide an indication of the potential susceptibility of an aquifer to contamination from other agricultural chemicals, such as atrazine. Similar relations between pesticide detection frequencies and nitrate concentrations have been documented in the literature (Koterba *et al.,* 1993; Kolpin *et al.,*1994), although nitrate has not always been found to be a reliable predictor of pesticide contamination (Barbash and Resek, 1996).

Atrazine detection frequencies were also found to exhibit a positive relation with the concentration of dissolved oxygen (DO; Figure 3B), in accord with similar correlations observed for ground water in Iowa (Kolpin *et al.,* 1997) and the northern midwest (Kolpin *et al.,* 1994). Because oxygen is consumed through both biotic and abiotic processes as ground water travels from the water table to greater depths, DO may provide a rough surrogate for ground-water residence time (Kolpin *et al.,* 1997). Previous research has shown substantial differences in median dissolved-oxygen concentrations between pre-1953 (0.14 mg/L) and post-1953 (1.46 mg/L) water (Kolpin *et al.,* 1997). The land-use studies with the highest dissolved-oxygen concentrations would therefore be those generally sampling the youngest (i.e., most recently recharged) ground water. This explanation for the observed relation between DO and atrazine detections during the land-use studies is consistent

Table 1. Ancillary Data Used in the Statistical Analysis to Determine Factors Significantly Related to the Occurrence of Atrazine and Metolachlor in Shallow Ground Water. These data were compiled from 50 land-use studies during the first phase of the National Water-Quality Assessment Program, 1993 to 1995.

Factor Name	**Factor Definition**	**Median Value**	**Spearman Rank Correlation Coefficients/ Significance Level (atrazine)**	**Spearman Rank Correlation Coefficients/ Significance Level (metolachlor)**
	LAND USE / LAND COVER (computed for 500-m buffer)* (U.S Geological Survey, 1990)			
CROP_PA	Percent of area in cropland and pasture	81.8	**0.357 / 0.011**	**0.469 / < 0.001**
ORCH_VI	Percent of area in orchards, groves, and vineyards	0.0	0.046 / 0.747	0.005 / 0.973
TFOR	Percent of area in forest	1.2	-0.216 / 0.353	0.129 / 0.371
TRANGE	Percent of area in rangeland	0.0	-0.169 / 0.241	-0.255 / 0.074
TWATER	Percent of area in water	0.0	0.082 / 0.569	-0.149 / 0.302
TWET	Percent of area in wetland	0.0	0.031 / 0.830	-0.001 / 0.995
	POPULATION (computed for 500-m buffer)* (U.S. Bureau of Census, 1991)			
POP90	Population (1990)	26.8	0.056 / 0.699	-0.055 / 0.703
	CLIMATE (computed for 500-m buffer)* (National Climatic Data Center, 1991)			
PRECI	Long-term mean annual precipitation (in/yr) (1951-80)	38.0	-0.029 / 0.842	0.220 / 0.124
TEMP	Long-term mean annual air temperature (°C) (1951-80)	10.8	**-0.351 / 0.012**	-0.101 / 0.485
	SOIL (computed for 500-m buffer)* (U.S. Department of Agriculture, 1994a)			
AWC	Available soil water capacity (in/in)	0.131	**0.408 / 0.003**	0.219 / 0.127
BDAV	Moist bulk density (g/cc)	1.43	-0.007 / 0.956	0.152 / 0.290
HYGP_A	Percent of area in hydrologic group A (high infiltration rate)	6.1	-0.066 / 0.646	-0.080 / 0.579
HYGP_B	Percent of area in hydrologic group B (moderate infiltration rate)	45.3	**0.327 / 0.020**	**0.281 / 0.048**
HYGP_C	Percent of land in hydrologic group C (slow infiltration rate)	21.1	0.022 / 0.878	-0.089 / 0.537
HYGP_D	Percent of land in hydrologic group D (very slow infiltration rate)	7.7	**-0.398 / 0.004**	**-0.350 / 0.013**
OMAV	Percent of average organic matter	0.6	0.168 / 0.244	0.064 / 0.659
SLOPE	Inclination of the land surface from horizontal	3.75	0.147 / 0.308	0.042 / 0.773
	HYDROGEOLOGY			
FRACT	Fractured aquifer (0 = no, 1 = yes)	0		
WDEPTH	Well depth below land surface (m)	10.9	**0.287 / 0.043**	-0.018 / 0.900
	AGRICULTURAL MANAGEMENT PRACTICES (computed for entire land-use study area)* (U.S. Department of Agriculture, 1994b)			
ARTI	Percent of area having artificial drainage	0.250	-0.099 / 0.492	0.129 / 0.371
IRRI	Percent of area using irrigation	0.992	0.097 / 0.502	-0.126 / 0.382
CTIL	Percent of area using conservation tillage	2.64	**0.383 / 0.006**	**0.336 / 0.017**
	PHYSICAL AND CHEMICAL DATA COLLECTED AT THE TIME OF SAMPLING			
pH	pH	7.21	0.172 / 0.232	0.005 / 0.970
DO	Dissolved-oxygen concentration (mg/L)	3.30	**0.486 / < 0.001**	**0.299 / 0.035**
FE	Dissolved-iron concentration (mg/L)	6.5	**-0.460 / < 0.001**	-0.211 / 0.141
TN	Total dissolved-nitrogen concentration (summation of nitrate + nitrate + ammonium) (mg/L)	2.53	**0.568 / < 0.001**	**0.331 / 0.014**
PHOS	Dissolved-phosphorus concentration (mg/L)	0.01	-0.115 / 0.424	**-0.359 / 0.010**
CL	Chloride concentration (mg/L)	14.8	0.237 / 0.097	0.144 / 0.319
	CHEMICAL USE (computed for 1000-m buffer)* (Gianessi and Anderson, 1996)			
AT_KG	Estimated agricultural use of atrazine (kg/year)	122.6	**0.449 / 0.001**	**0.668 / < 0.001**
MET_KG	Estimated agricultural use of metolachlor (kg/year)	202.6	**0.483 / <0.001**	**0.697 / < 0.001**

*Mean values for wells in land-use study.

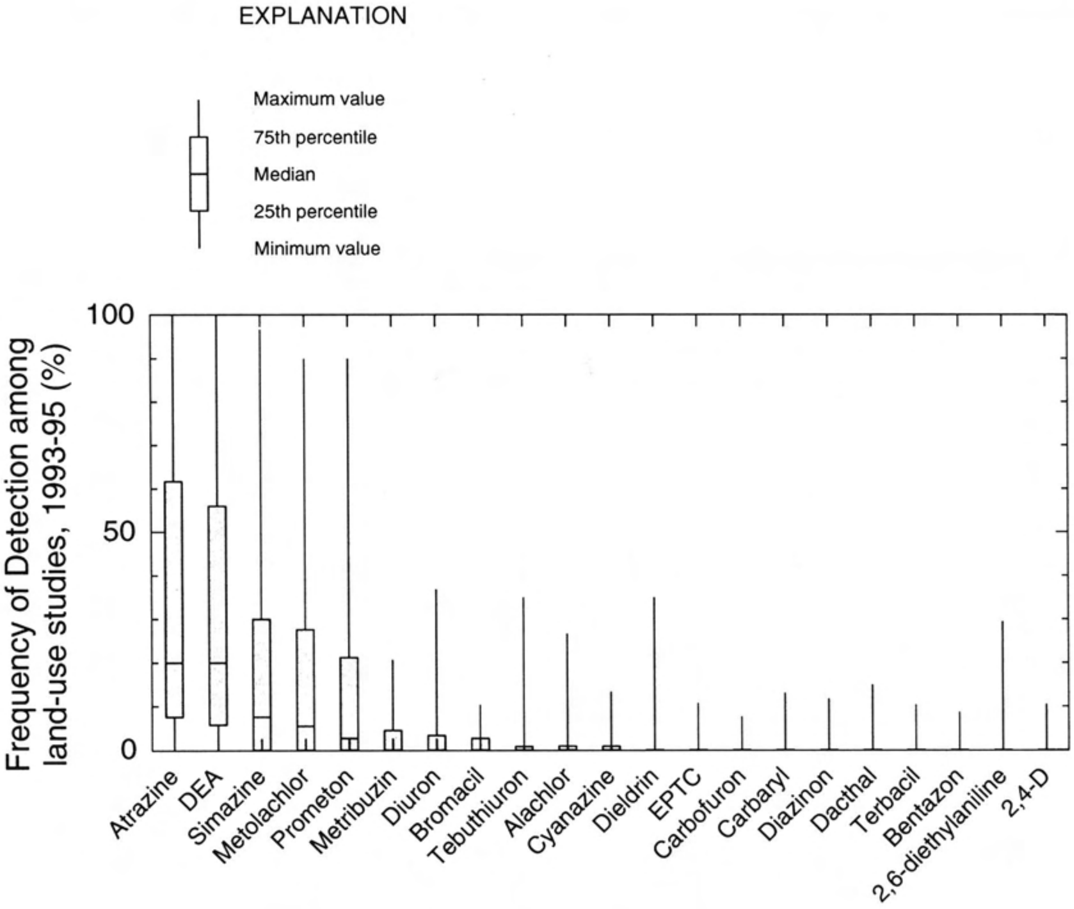

Figure 2. Most Frequently Detected Pesticide Compounds in Shallow Ground Water From the 50 NAWQA Land-Use Studies, 1993 to 1995.

with results from previous investigations (Kolpin *et al.,* 1995; Saad and Thorstenson, 1998; Shedlock *et al.,* 1999) that have shown pesticide detections, in general, to be more likely in younger ground water. Similarly, because the water-soluble form of iron (ferrous ion) is stable only under hypoxic conditions (i.e., in the absence of detectable dissolved oxygen), the inverse relation between atrazine detection frequencies and iron concentrations (FE; Figure 3C) may also reflect an inverse relation between ground-water residence time and the likelihood of pesticide detection.

The frequency of atrazine detection was found to be directly related to the estimated agricultural use of atrazine (AT_KG; Figure 3D). Positive relations with use have also been documented by other studies for atrazine (Kolpin *et al.,* 1994; Barbash and Resek, 1996; Saad and Thorstenson, 1998; Ferrari and Denis, 1999). It is interesting to note, however, that the frequencies of atrazine detection were more strongly related to indicators of ground-water residence time (DO and FE) or susceptibility to surface-derived contamination (TN) than to atrazine use (AT_KG). This may be a consequence of the wide use of atrazine in both agricultural and nonagricultural settings (Gianessi and Anderson, 1996; Barbash *et al.,* 2001). Had it been possible to account for the nonagricultural use of atrazine, a stronger relation between the intensity of its use and the frequency of its detection may have been observed.

The available water-holding capacity of the soil (AWC), was found to be positively related to the frequencies of atrazine detection (Figure 3E). This result was unexpected because it was anticipated that soils with lower AWC (sandier soils) would correspond to greater frequencies of atrazine detection. Soils with the potential to hold more water, however, tend to have longer periods of saturation that often lead to the development of hypoxic conditions. Thus, the relation with AWC shown in Figure 3E might be a consequence of the fact that atrazine transformation rates have been observed to be slower under hypoxic than under aerobic conditions (Kaufman and Kearney, 1970; Nair and Schnoor, 1992; Agertved *et al.,* 1992). This hypothesis, however, is inconsistent with the

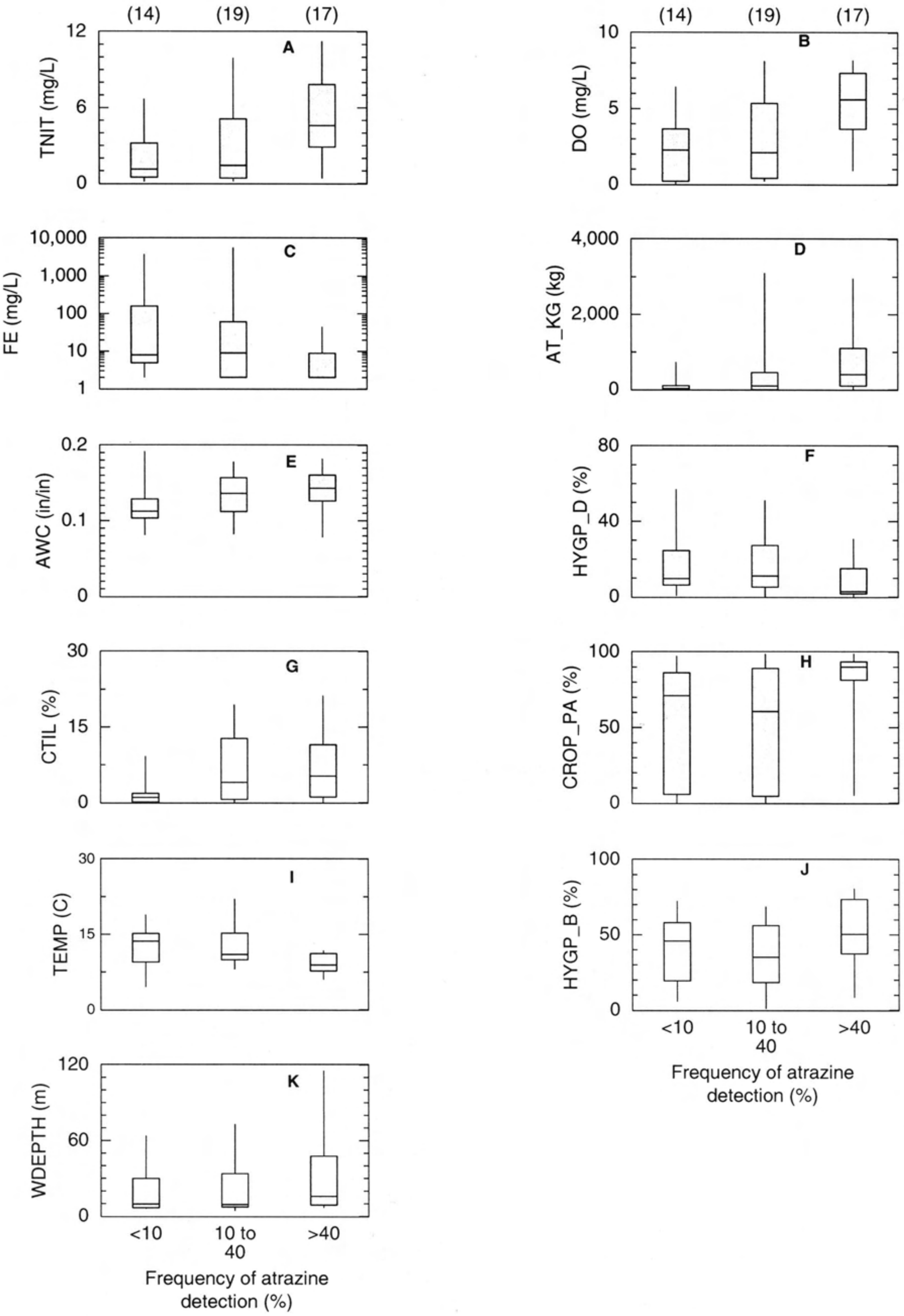

Figure 3. Factors With the Most Significant Correlation to the Frequency of Atrazine Detection in Shallow Ground Water Among the NAWQA Land-Use Studies, 1993 to 1995. Factor definitions, Spearman rank correlation coefficients, and significance levels are provided in Table 1. See Figure 2 for the explanation of a boxplot. Number in parentheses denotes the number of land-use studies.

direct relation observed between atrazine detection frequencies and DO (Figure 3B). The observed relation to AWC might also result from the fact that this parameter can provide an indication of soils appropriate for growing crops. Consistent with this possibility, a significant direct relation (P = 0.016) was observed between AWC and the amount of cropland and pasture within the vicinity of the sampled wells (CROP_PA) .

HYGP_D, the amount of land in hydrologic group D (USDA, 1994a), was found to be inversely related to frequencies of atrazine detection (Figure 3F). The HYGP_D soils exhibit very slow infiltration rates (USDA, 1994a), and therefore tend to impede the downward movement of surface-derived solutes, as well as water. These soils are also more likely to be artificially drained to increase crop production, diverting atrazine and other applied chemicals to nearby streams and thus reducing the likelihood of these solutes reaching ground water. This relation is consistent with observations from other studies documenting lower concentrations of agrichemicals in ground water beneath agricultural areas with less permeable soils (Burkart *et al.,* 1999a; Nolan *et al.,* 1997; Fenelon and Moore, 1998; Nolan and Stoner, 2000).

The amount of land in conservation tillage, CTIL, was positively related to the frequencies of atrazine detection (Figure 3G). This relation may be a consequence of increased pesticide application rates (Day *et al.,* 1999), an increase in macropore flow because more of the soil structure remains intact when tillage is diminished (Barbash and Resek, 1996; Flury, 1996), or a combination of these two effects. As discussed above, the amount of atrazine used directly affects atrazine transport to ground water. In addition, an increase in the abundance of macropores such as earthworm burrows, soil fractures, and voids formed by decaying crop roots serve as preferential flow paths which can rapidly transport atrazine to ground water (Flury, 1996; Sadeghi and Isensee, 1994; Sigua *et al.,* 1995).

The percent of land in cropland and pasture, CROP_PA, was also found to be positively related to atrazine detection (Figure 3H). Because it quantifies land use rather than chemical applications, this parameter provides an indication of potential, rather than actual atrazine use. It is therefore not surprising that this surrogate for atrazine use was less strongly related to atrazine detection frequencies than was estimated agricultural use of atrazine (AT_KG).

The mean annual air temperature (TEMP), was inversely related to atrazine detection (Figure 3I). This parameter also provides a relative indication of the mean annual soil temperatures (for which national data were not available) for an area. Thus, the observed relation may be a simple consequence of the fact that the rate of atrazine transformation increases with increasing soil temperatures (Koskinen and Clay, 1997).

HYGP_B, the amount of land in hydrologic group B (USDA, 1994a), was found to be positively related to the frequency of atrazine detection (Figure 3J). The HYGP_B soils are those with moderate infiltration rates (USDA, 1994a) that readily transmit water (and thus atrazine) through the soil zone to the subsurface. The relation in Figure 3J is consistent with previous research demonstrating that the downward movement of atrazine is higher in soils that are more permeable (Koskinen and Clay, 1997).

The depth of the sampled wells (WDEPTH), was found to be positively related to the frequency of atrazine detection (Figure 3K). By contrast, numerous other studies have observed inverse relations between well depths and the frequencies of pesticide occurrence (e.g., USEPA, 1992; Klaseus *et al.,* 1988; Kolpin *et al.,* 1997). The unexpected positive relation between atrazine detection frequencies and well depth for this study may have been caused by the fact that the land-use studies were designed to focus on shallow groundwater (well depths for the 50 land-use studies used in this statistical analysis: 25th percentile = 7.8 m, median = 10.9 m , and 75th percentile = 45.3 m). Previous research has shown that areas with permeable surficial deposits generally have deeper water tables (Saad, 1997). Indeed, a significant positive relation ($P < 0.001$) was observed between WDEPTH and HYGP_B. Thus, for this study of shallow groundwater, WDEPTH may be providing an indication of the relative permeability of the surficial materials (similar to HYGP_B above).

To identify the set of factors that best explained the variability in the frequencies of atrazine detection among the 50 land-use studies, a multiple regression analysis was conducted using all available ancillary factors. From this analysis, the regression equation that best explained the variability in the frequencies of atrazine detection was as follows:

$$6.13 + 5.01(\mathrm{AWC}) + 0.21(\mathrm{AT\_KG}) + 0.72(\mathrm{TN}) + 0.37(\mathrm{TWATER}). \quad (1)$$

The R^2 for this model was 0.447. The percent of area in water near sampled wells (TWATER) was the only factor not identified as significant in the univariate analysis. The relation between atrazine detection frequency and TWATER may reflect the transport of atrazine from processes such as episodic stream flooding (Squillace *et al.,* 1996), bank storage of stream water (Squillace,1996), streams losing water to the ground-water system (Burkart *et al.,* 1999b), or induced infiltration of river water to pumping wells (Boyd, 2000; Duncan *et al.,* 1991). Previous research has also documented a direct relation between the frequencies of herbicide detection and the proximity of the sampled wells to streams (Kolpin *et al.,* 1994). Improvements in the quality and accuracy of the data used for this study, and the inclusion of additional explanatory variables, are expected to capture some of the remaining 55 percent of the variance in atrazine detection frequencies left unexplained by the present analysis.

Metolachlor

The factors found to exhibit statistically significant nonparametric correlations with the frequency of metolachlor detection for the 50 land-use studies are shown in Figure 4 and Table 1. With the exception of phosphorous concentration (PHOS), all factors that were significantly related to the frequencies of metolachlor detection (Figure 4) also correlated with atrazine detections (Figure 3). Because phosphorous has a strong affinity to sorb to clay particles, PHOS may provide an indication of relative soil infiltration rates for an area (higher PHOS indicating more rapid

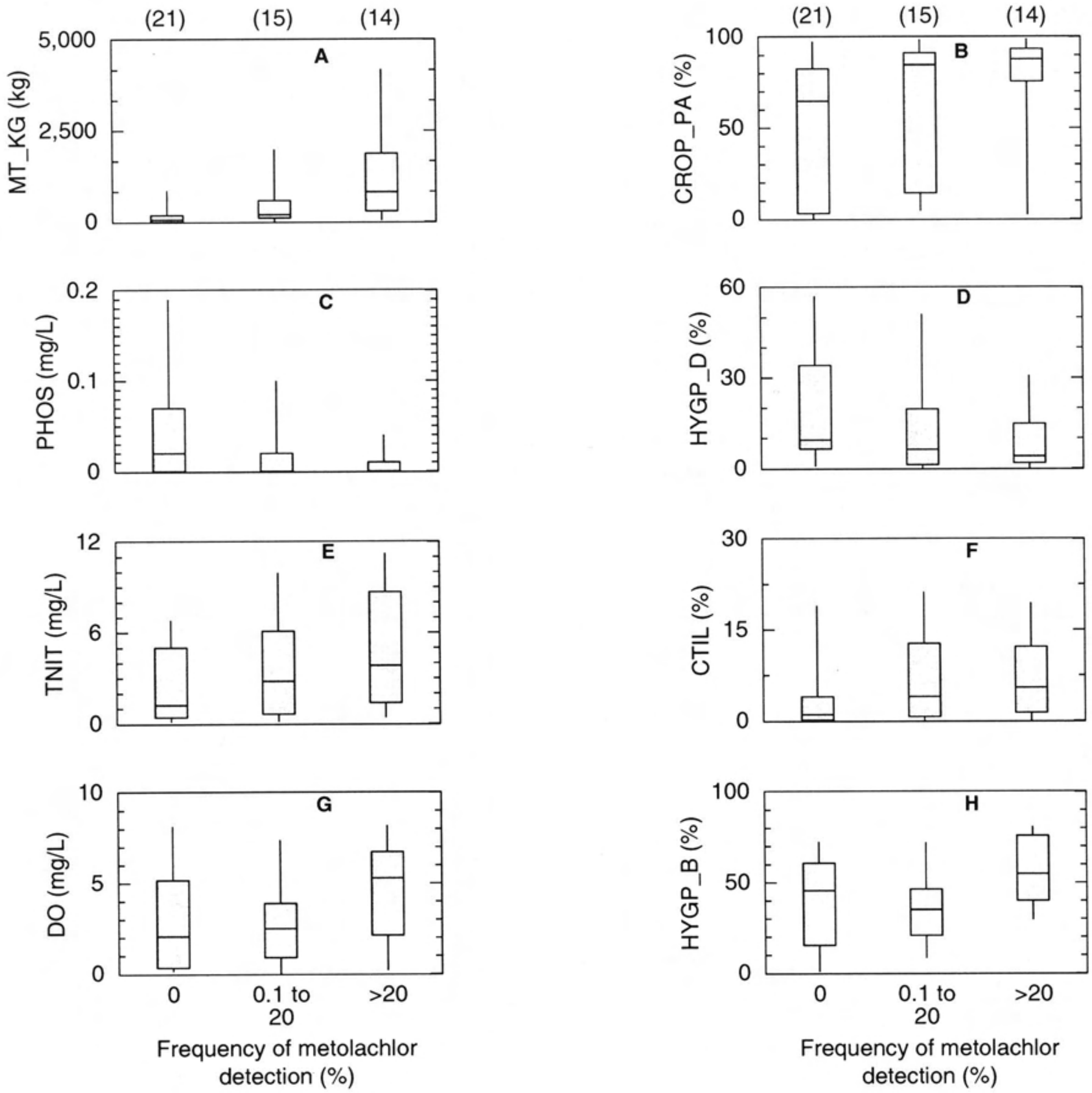

Figure 4. Factors With the Most Significant Correlation (Spearman's rank) to the Frequency of Metolachlor Detection in Shallow Ground Water Among the NAWQA Land-Use Studies, 1993 to 1995. Factor definitions, Spearman rank correlation coefficients, and significance levels are provided in Table 1. See Figure 2 for the explanation of a boxplot. Number in parentheses denotes the number of land-use studies.

soil infiltration rates). Indeed, a significant direct relation (P = 0.004) was observed between PHOS and HYGP_D.

While the factors that were most strongly correlated with frequencies of atrazine detection (Figure 3, Table 1) were those providing general indications of the susceptibility of ground water to surface-derived contamination (TN) and ground-water age (DO, FE), the frequencies of metolachlor detection were most strongly correlated with parameters that are either directly (MET_KG) or indirectly (CROP_PA) related to its agricultural use (Figure 4, Table 1). This contrast between the sets of factors that were most strongly correlated with the frequencies of detection of the two herbicides appear to be related largely to the fact that a much smaller proportion of total metolachlor use in the United States takes place in nonagricultural areas than is the case for atrazine (Barbash *et al.,* 1999). Thus, MET_KG likely is a better estimation of the total metolachlor use than AT_KG is for total atrazine use. If pesticide use data incorporated reliable estimates of nonagricultural use, estimated use may have had the strongest correlation to frequencies of detection for both metolachlor and atrazine.

To identify the set of factors that best explained the variability in the frequencies of metolachlor detection among the 50 land-use studies, a multiple regression analysis was conducted using all available ancillary factors. From this analysis, the regression equation that best explained the variability in the frequencies of metolachlor detection was as follows:

$$1.83 + 0.62(\mathrm{MET\_KG}) - 2.33(\mathrm{WDEPTH}) + 1.09(\mathrm{TN}) + 1.85(\mathrm{FRACT}). \quad (2)$$

The R^2 for this model was 0.544. Although a greater portion of variance in detection frequencies was captured for metolachlor than for atrazine, about 46 percent of the variance in metolachlor detection frequencies was still left unexplained by the set of factors examined. WDEPTH and the presence of a fractures in the aquifer (FRACT) were factors not identified as significant in the univariate analysis.

CONCLUSIONS

In an effort to obtain a better understanding of the occurrence of pesticides in shallow ground water on a national scale, a statistical analysis was conducted to determine significant relations between explanatory variables (a set of 30 factors that potentially affect the source, fate, or transport of pesticides) to the occurrence of atrazine and metolachlor in ground water using water-quality data from the first group of NAWQA land-use studies (1993 to 1995). Atrazine and metolachlor were selected for this study because they were detected with a wide range of frequencies in ground water during the first phase of NAWQA, but have differing chemical and physical properties.

While the factors that were most strongly correlated with frequencies of atrazine detection in shallow ground-water networks were those providing general indications of the susceptibility of ground water to surface-derived contamination (TN) and ground-water age (DO, FE), the frequencies of metolachlor detection were most strongly correlated with factors that estimated (MET_KG) or indicated (CROP_PA) the intensity of the agricultural use of metolachlor. Because detailed use estimates for these compounds are currently available only for agricultural settings, this contrast appears to be related largely to the fact that a much smaller proportion of total metolachlor use in the United States takes place in nonagricultural areas than is the case for atrazine. As a result, the estimates of agricultural applications provide a less reliable indication of total chemical use for atrazine than for metolachlor. Had the use data incorporated reliable estimates of nonagricultural use, use estimates may have had the strongest correlation to frequencies of detection for both metolachlor and atrazine.

A multivariate analysis demonstrated that the factors of interest explained about 50 percent of the variance in atrazine and metolachlor detection frequencies among the NAWQA land-use studies examined. The estimate of use for the respective chemical and TN were factors identified in the multivariate analysis for both atrazine and metolachlor. The inclusion of other factors related to pesticide fate and transport in ground water, or improvements in the quality and accuracy of the data employed for the factors examined, may capture more of the remaining variance in the frequencies of atrazine and metolachlor detection.

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