7 Prediction Where Data are Inadequate

Strategies for managing pesticides require far more information than we can afford to directly measure for all the places, times, and pesticides of interest. In addition, many strategic decisions—such as setting monitoring priorities, approving a pesticide registration, and determining how much to spend on a management strategy—inherently depend on predicting the potential effects of pesticides on water quality for locations that have never been directly assessed. In these situations, statistical models and other types of models can be useful for predicting water-quality conditions at unmonitored locations under a range of possible circumstances. Such tools are essential for efficient water-quality management.

Photograph by Albert E. Becher

In this chapter, three examples illustrate the development of statistical models from NAWQA data and some of the ways in which the models can be applied to national-scale analysis of water-quality conditions.

Approach to Prediction

NAWQA pesticide data collected from 1992 to 2001 support the development and testing of a wide range of models, particularly statistical models. Statistical models have been developed by NAWQA to predict pesticide levels in streams and ground water for locations where pesticide concentrations have not been measured. This expansion of water-quality assessment from individual monitoring sites to unstudied locations by use of models for prediction, or spatial extrapolation, is fundamental to extending the targeted local and regional studies of NAWQA to a comprehensive national assessment (Alaska and Hawaii have not been included in these models because there are no suitable pesticide-use data for these States).

The NAWQA statistical models for pesticides use linear regression methods to establish quantitative linkages between pesticide concentrations measured at NAWQA sampling sites and a variety of anthropogenic (human-related) and natural factors that affect pesticides. Such factors include pesticide use, soil characteristics, hydrology, and climate—collectively referred to as explanatory variables. Model-development data consist of measured pesticide concentrations or detection frequencies, together with the associated values of the explanatory variables for the sampling sites. The models are built using the explanatory variables that best correlate with, or explain, the concentrations or frequencies of occurrence of pesticides observed in streams and ground water. Although explanatory variables included in the models are significantly correlated with pesticide concentrations or detection frequencies, the specific cause-and-effect relations responsible for the observed correlations are not always clear, and inferences regarding causes should be considered as hypotheses.

In developing the pesticide models, all potential explanatory variables were required to have values available from existing data sources for all locations in the conterminous United States, so that national extrapolation would be possible (the only exception, as explained below, was fish lipid content for the dieldrin model). Overall, 30 to 60 possible variables were considered, depending on the specific model; these were reduced to the 4 to 6 explanatory variables that were most significant and yielded optimal model formulations. Each model incorporates an uncertainty analysis, which allows assessment of the reliability of the model predictions and also the expression of model predictions as probabilities that concentrations will exceed a specific value, such as a water-quality benchmark, at a particular location.

The three NAWQA models and nationally extrapolated results presented in this chapter are those developed for (1) concentrations of atrazine in stream water; (2) concentrations of dieldrin in whole fish; and (3) detection frequencies for atrazine in shallow ground water underlying agricultural settings. The extrapolations for atrazine concentrations in stream water and dieldrin concentrations in fish tissue are for streams included in the USEPA River Reach file (Nolan and others, 2003), which includes more than 600,000 miles of streams and more than 60,000 individual stream reaches with watersheds. The extrapolations of detection frequencies for atrazine in shallow ground water were made for all areas of the Nation where at least 50 percent of the land is in agricultural use. More detailed information on model development methods and supporting data, as well as uncertainty analyses, are provided by Larson and others (2004), Nowell and others (2006), and Stackelberg and others (2006). Additional work is currently underway on (1) a multi-pesticide model for stream water that incorporates selected chemical and physical properties of each compound, (2) expanding the models for fish tissue to include additional organochlorine compounds, and (3) site-specific, concentration-based models for atrazine in ground water.

Atrazine Concentrations in Streams

Model predictions of atrazine levels in streams across the Nation show the highest annual mean concentrations throughout the high-use areas of the Corn Belt and the Mississippi Valley and Delta regions, and in some areas of Texas, Pennsylvania, and Maryland. Figure 7–1 shows measured concentrations used to develop the model and figure 7–2 shows predicted concentrations. As noted along with other model details in the accompanying sidebar (p. 121), the model is based on the time-weighted annual mean for each model-development site. Annual means for a few streams in the Ohio and Mississippi Valleys and in southern Louisiana are predicted to exceed 3 μg/L, the human-health benchmark used for atrazine (Chapter 6 and Appendix 3A). The benchmark for atrazine is the USEPA MCL for drinking water. As a drinking-water standard, the MCL applies to finished water in public water supplies, whereas the predictions shown in figure 7–2 are for untreated stream water. Comparisons of model predictions with human-health benchmarks, however, serve as screening-level assessments of the suitability of potential drinking-water sources, as discussed in Chapter 6.

For more than half of the streams with a predicted annual mean atrazine concentration exceeding 0.3 µg/L (fig. 7–2), there is at least a 5-percent chance that the actual annual mean concentrations will exceed the human-health benchmark of 3 µg/L (fig. 7–2). Model estimates of probabilities shown in figure 7–2 indicate that at least 1 out of 20 (5 percent) of the streams shown in yellow, orange, or red would be expected to have annual mean atrazine concentrations greater than 3 µg/L. These streams may not be suitable as sources of drinking water without treatment or other management strategies to reduce atrazine concentrations. The streams with a greater than 5-percent probability of exceeding the benchmark represent about 7 percent of the Nation's stream miles (45,704 of 649,935 mi). Approximately 192 stream miles (less than 1/10th of 1 percent of the Nation's stream miles) are predicted to have more than a 50-percent probability of exceeding 3 µg/L.

The model indicates that atrazine use intensity is the most important factor explaining atrazine concentrations in streams—the more intensive the use of atrazine in a watershed, the higher the atrazine concentration in the stream. Specifically, estimated atrazine use intensity within each watershed explains 64 percent of the variance in annual mean atrazine concentrations in streams across the Nation. Four additional variables explain another 13 percent of the variability, most of which is accounted for by rainfall erosivity and soil erodibility—factors used in the revised Universal Soil Loss Equation (Renard and others, 1997). Rainfall erosivity and soil erodibility quantify, respectively, the energy of storms in a specific area (averaged over several years), and the susceptibility of soils to erosion by runoff. As these two factors increase, atrazine concentrations also increase, indicating that transport of atrazine is highest in areas of high-energy rain storms and in areas where soils are most susceptible to erosion. Alternatively, soil erodibility may indicate high surface runoff, rather than actual transport of atrazine with soil particles. Overall, the complete model explains a total of 77 percent of the variance in observed annual mean atrazine concentrations.

Development and Application of the Atrazine Model for Stream Water

As described by Larson and others (2004), the model for estimating atrazine concentrations in streams is based on time-weighted annual mean concentrations measured by NAWQA from 1992 to 2001 at 112 sites (fig. 7–1). The single most complete year of data was used to calculate the annual mean concentration for each site. The predicted values in figure 7–2 are median estimates of the annual mean, such that 50 percent of the actual annual means are expected to be greater than, and 50 percent less than, the predicted value. Nonagricultural uses of atrazine are not included and, as a result, predictions may represent underestimates for watersheds with substantial nonagricultural use. To illustrate a practical example of how such models can be applied to water-quality assessment, model estimates are compared with the human-health benchmark for atrazine, USEPA's Maximum Contaminant Level (MCL) for drinking water (Chapter 6 and Appendix 3). The model also was used to estimate the probability, after accounting for model uncertainty, that any particular stream site may have an annual mean atrazine concentration greater than 3 µg/L (fig.7–2).

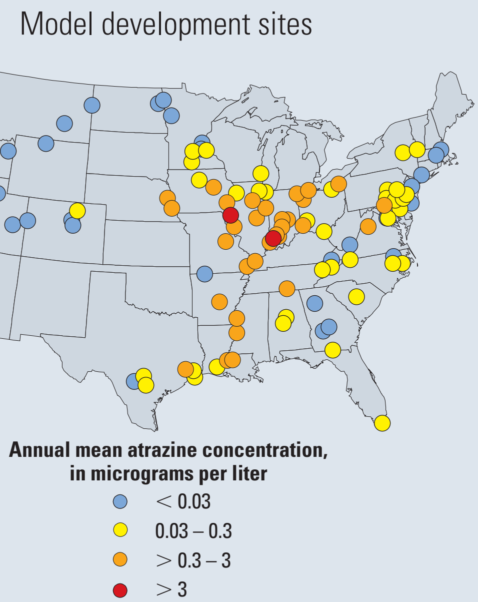
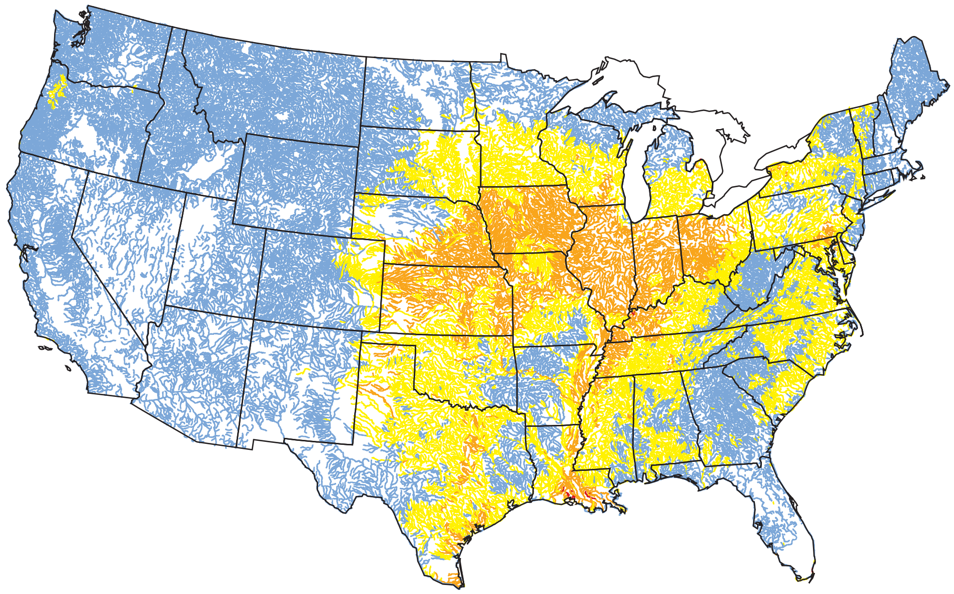


Figure 7–1. The model for annual mean concentrations of atrazine in streams was developed from data for 112 sites distributed across the country, which represent a wide range of hydrologic settings and atrazine concentrations.

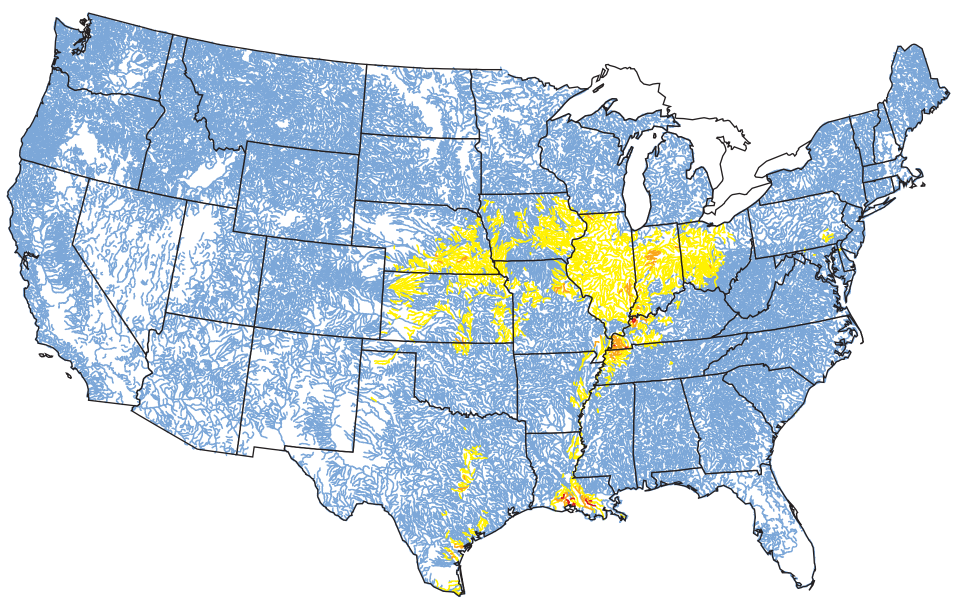
Predicted annual mean concentration of atrazine in streams



Predicted annual mean concentration of atrazine, in micrograms per liter

< 0.03
0.03 – 0.3
> 0.3 – 3
> 3

Probability of exceeding the human-health benchmark for atrazine



Probability of exceeding 3 micrograms per liter

< 5%
5 – 25%
> 25 – 50%
> 50%

Figure 7–2. Model predictions of annual mean atrazine concentrations in streams across the Nation show the highest concentrations (orange and red streams) throughout the high-use areas of the Corn Belt and the Mississippi Valley, and in some areas of Texas, Pennsylvania, and Maryland. Model predictions of the probability that atrazine concentrations are greater than the human-health benchmark of 3 µg/L for drinking water indicate that many streams in the Corn Belt and Mississippi Valley and Delta regions have greater than a 5-percent probability of having annual mean concentrations greater than the benchmark.

Dieldrin Concentrations in Fish

Model predictions of dieldrin concentrations in whole fish show the highest concentrations in the Corn Belt—especially in Illinois—where aldrin was heavily used on cropland. Figure 7–3 shows measured concentrations used to develop the model and figure 7–4 shows predicted concentrations. Dieldrin is an organochlorine compound that was used as an insecticide until its agricultural use was discontinued in the early 1970s, and it is also a degradate of aldrin, another insecticide that was used for agricultural purposes through the early 1970s. As noted along with other model details in the accompanying sidebar, model predictions are for fish with a 6.2 percent lipid content, the national average lipid content for all whole fish sampled. Most streams that are predicted to have a dieldrin concentration greater than 25 µg/kg (micrograms per kilogram of fish tissue, wet weight) also have a 5 percent or greater chance (more than 1 in 20) of exceeding 120 µg/kg (fig. 7–4), which is a wildlife benchmark for dieldrin in fish tissue (120 µg/kg is the highest of the dieldrin benchmarks compiled for this report; see Chapter 6 and Appendix 3B). These streams represent about 6 percent of the Nation's stream miles (40,222 out of 649,935 mi). Approximately 627 stream miles (about 1/10th of 1 percent of the Nation's stream miles) are predicted to have a 50-percent or greater probability of exceeding the dieldrin wildlife benchmark of 120 µg/kg.

The dieldrin model indicates that the amount of forested land in a watershed is the most important factor explaining the concentrations of dieldrin observed in fish—the greater the proportion of forested land (where historical use would have been least), the lower the dieldrin in fish tissue. Fish lipid content was also an important variable, which is consistent with the fact that organochlorine pesticides are hydrophobic compounds, which have a strong affinity for lipids, and thus tend to accumulate in high-lipid tissues. Two additional factors in the dieldrin model that, like forested land, are related to past use of dieldrin and aldrin represent (1) the estimated historical use of the compounds in agriculture and (2) their use for termite control. Dieldrin concentrations decrease with increasing amounts of forested land and increase with increasing historical use in agriculture or for termite control. Together, these three use-related factors and lipid content explain 58 percent of the variability in dieldrin concentrations measured in whole fish in streams across the Nation. With the addition of two other less influential variables, the complete model explains 64 percent of this variability.

Development and Application of the Dieldrin Model for Whole Fish

As described by Nowell and others (2006), the model for estimating dieldrin concentrations in fish is based on concentrations measured in whole fish sampled by NAWQA from 1992 to 2001 at 648 sites across the country. The 514 sites shown in figure 7–3 are limited to the subset of model development sites with whole-fish samples having 2.3–10.4 percent lipid content (the lowest and highest 10 percent of lipid levels were excluded from the map, but not model development). One composite sample (each composed of 5–10 fish of a single species) was collected at each site. The national data include 59 different species of fish, most frequently common carp (29 percent of samples) and white sucker (26 percent). One effect of compositing is to reduce variability in contaminant concentrations caused by differences in age and size among individual fish. An important explanatory variable in the dieldrin model is fish lipid content, which is not nationally available for all streams because it is a characteristic of the fish, rather than the stream or watershed. The inclusion of fish lipid content in the model accounts—to some extent—for differences among fish in age, size, and species because lipid content generally varies among species and increases (within a species) with increasing fish age and size (Nowell and others, 1999).

Model predictions were made using the national average lipid content for whole fish, which was 6.2 percent for samples collected by NAWQA and the U.S. Fish and Wildlife Service (Schmitt and Bunck, 1995). Predicted concentrations of dieldrin in fish, shown in figure 7–4, are median estimates for fish with 6.2 percent lipid content. Consequently, actual concentrations are expected to be lower than the predicted value at 50 percent of sites and higher at 50 percent of sites. Also, fish with lipid content greater than 6.2 percent would likely have higher dieldrin concentrations, and fish with lower lipid content would likely have lower dieldrin concentrations, than those shown in figure 7–4. As examples, lipid content values typical of common fish species in the United States are lake trout, 15 percent; channel catfish, 7.5 percent; common carp, 6.5 percent; white sucker, 5.8 percent; largemouth bass, 4.2 percent; and bluegill, 3.1 percent. See Nowell and others (2006) for further discussion of uncertainty in model predictions.

To illustrate a practical example of how such models can be applied to water-quality assessment, model estimates are compared with the New York guideline for the protection of fish-eating wildlife, which was the highest wildlife benchmark compiled for dieldrin in fish tissue (Chapter 6 and Appendix 3B). The model also was used to estimate the probability, after accounting for model uncertainty, that any particular stream site may have a dieldrin concentration greater than 120 µg/kg in whole fish with a 6.2 percent lipid content (fig. 7–4).

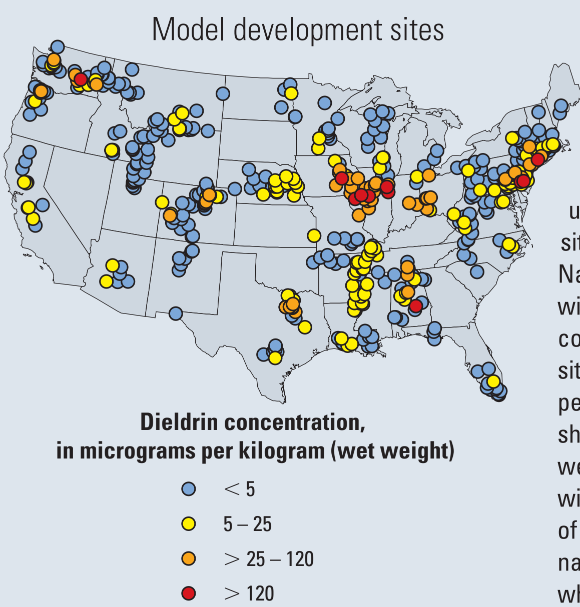
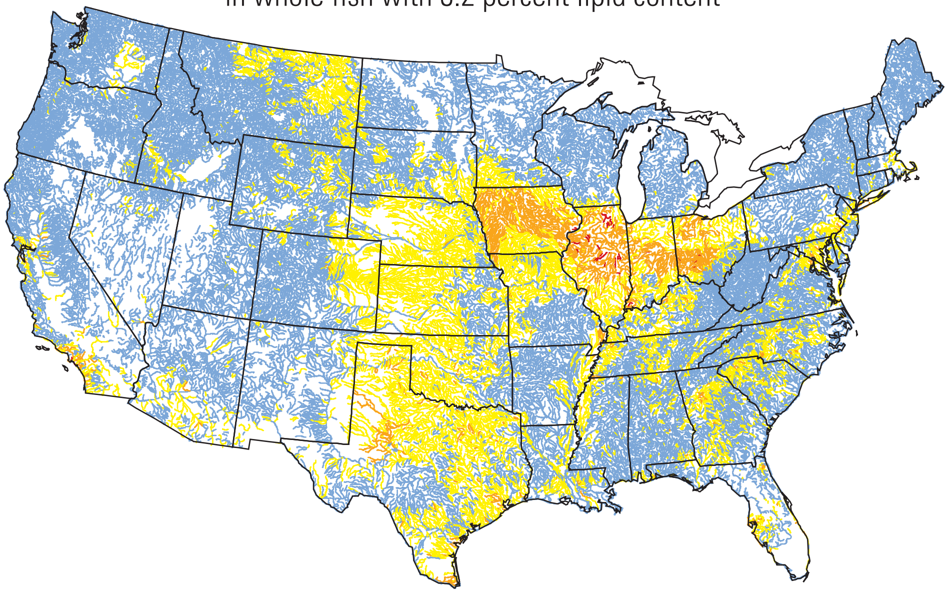


Figure 7–3. The model for dieldrin concentrations in whole-fish tissue was developed using data from 648 sites throughout the Nation, representing a wide range of dieldrin concentrations (514 sites with 2.3–10.4 percent fish lipid are shown). Predictions were made for fish with a lipid content of 6.2 percent, the national average for whole fish.

Predicted dieldrin concentrations
in whole fish with 6.2 percent lipid content



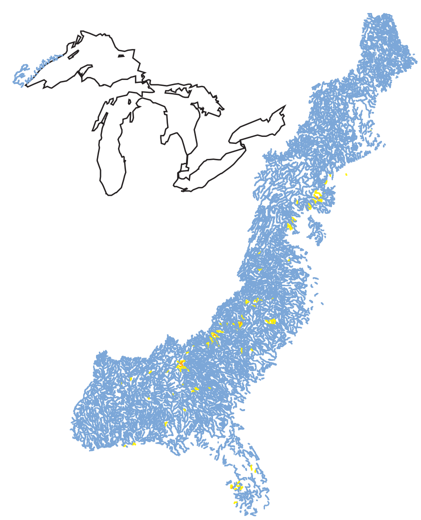
Predicted dieldrin concentration, in micrograms per kilogram (wet weight)

< 5

5 – 25

> 25 – 120

> 120



Probability of exceeding 120 micrograms per kilogram

Figure 7–4. Model predictions of dieldrin concentrations in whole fish in streams across the Nation show the highest concentrations in the Corn Belt, particularly Illinois, where aldrin (which degrades to dieldrin) was heavily used on cropland. Model predictions of the probability that dieldrin concentrations exceed the wildlife benchmark of 120 µg/kg indicate that there is greater than a 5-percent probability in many Corn-Belt streams that whole fish (with 6.2 percent lipid) contain dieldrin concentrations that exceed the benchmark.

Atrazine Detection Frequencies in Shallow Ground Water

Model predictions show that the highest frequencies of atrazine detection in shallow ground water beneath agricultural areas are expected in parts of the western Corn Belt, eastern Great Plains, Pacific Northwest (eastern Washington), and Mid-Atlantic regions (especially southeastern Pennsylvania). Figure 7–5 shows measured detection frequencies used to develop the model and figure 7–6 shows predicted detection frequencies for each square kilometer of land with 50 percent or more agricultural land. The areas with the highest frequencies of detection are those with relatively high atrazine use in hydrologic settings that also favor the transport of pesticides to ground water.

In contrast to the model for atrazine concentrations in stream water, atrazine use is not the most important factor for predicting atrazine occurrence in ground water. This finding is consistent with results from an earlier study of relations between atrazine in ground water and various land-use factors by Kolpin (1997), in which atrazine use was not found to be significantly correlated with atrazine occurrence in ground water. In the model presented herein, atrazine use explains only about 7 percent of the overall variability in the frequency of its detection in ground water. The two most important factors were found to be the proportion of land with subsurface tile drain systems and other artificial drainage, and the average vertical permeability of soil, which together explain 48 percent of the variability in atrazine detection frequencies. As the amount of artificial drainage increases, predicted detection frequencies decrease—a finding consistent with the fact that artificial drainage systems divert water and pesticides away from the ground-water system. Conversely, as the average vertical permeability of soils increases, predicted detection frequencies also increase because water and pesticides at the land surface are more likely to move vertically to ground water in areas with high-permeability soils. The influential role of these factors is particularly evident in Indiana and Ohio, where atrazine use is intense, but NAWQA studies, like several other previous studies (Barbash and Resek, 1996), found relatively low atrazine detection frequencies in ground water. Soils in these areas tend to be poorly drained and require artificial drainage to dewater the agricultural fields, thus reducing atrazine transport to ground water. With the addition of two other less influential variables, the complete model explains 58 percent of the variability in atrazine detection frequencies observed in shallow ground water beneath the agricultural areas studied.

Development and Application of the Atrazine Model for Ground Water

As described by Stackelberg and others (2006), the model for predicting atrazine occurrence in shallow ground water within agricultural areas is based on the frequencies of detection measured by NAWQA from 1992 to 2001 in 52 studies, each of which sampled about 20 to 30 shallow wells in agricultural areas (fig. 7–5). The model was used to predict the frequency of atrazine occurrence in shallow ground water in agricultural areas of the United States (fig. 7–6). Predictions were made for each 1 square kilometer area with 50 percent or more agricultural land use. Nonagricultural use of atrazine was not included in use estimates, and thus, predictions may underestimate occurrence in areas where nonagricultural use is substantial.

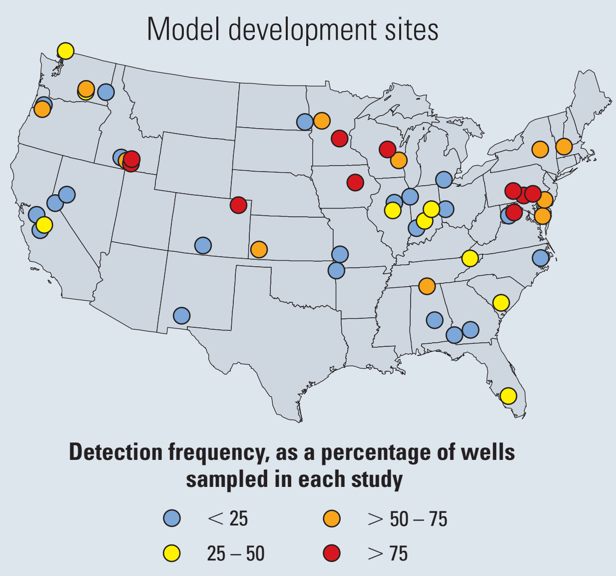


Figure 7–5. The model for atrazine occurrence in shallow ground water within agricultural areas was developed from frequencies of detection in wells sampled for studies of shallow ground water in 52 agricultural areas across the country. The ground-water studies represent a wide range of agricultural and hydrologic settings, as well as atrazine detection frequencies.

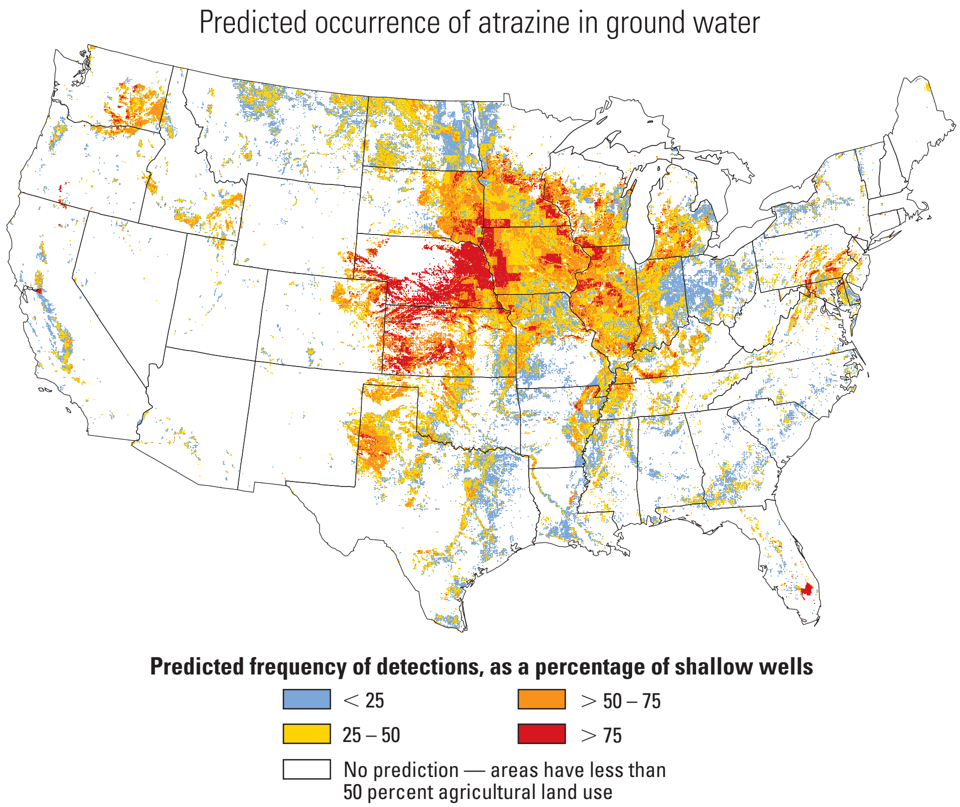


Figure 7–6. Model predictions show that the highest frequencies of atrazine detection in shallow ground water beneath agricultural areas are expected in parts of the western Corn Belt, eastern Great Plains, Pacific Northwest (eastern Washington), and Mid-Atlantic regions (especially southeastern Pennsylvania). These areas represent relatively high atrazine use in hydrologic settings that favor the transport of pesticides to ground water.