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Nitrate in Ground Water:

Using a model to simulate the probability of nitrate contamination of shallow ground water in the conterminous United States — Supplementary information

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Ground water is a critical national resource that can be degraded by elevated levels of nitrate

More than 43 million people in the United States are served by self-supplied domestic water systems, and almost all (98 percent) of this water comes from ground water. Ground water also is the source of water for about 90 million people who are served by public water-supply systems. Unfortunately, shallow ground water (typically less than about 5 meters deep in this study) is susceptible to contamination by chemicals derived from the land surface. One such chemical often derived from the land surface is nitrate, which dissolves easily in water. As water infiltrates downward, nitrate is readily transmitted through soil and can seep into ground water.

Nitrate, from both natural sources and human activities, is possibly the most prevalent contaminant in ground water, and can persist in shallow ground water for years under well-oxygenated conditions. About 13 percent of shallow wells sampled beneath agricultural and urban land-use study areas as part of the National Water-Quality Assessment (NAWQA) Program during 1992–99 exceeded the U.S. Environmental Protection Agency's drinking-water standard for nitrate (10 milligrams per liter). Shallow ground water in relatively undeveloped areas of the United States contains about 1 milligram per liter (mg/L) of nitrate (Nolan and Hitt, 2003).

Contamination of shallow ground water used as drinking water is a public-health concern. Shallow ground water is more susceptible to nitrate contamination than deep ground water, and domestic wells typically are shallower than public-supply wells; shallow domestic wells are not routinely monitored for water quality. Even if people do not drink shallow ground water in a particular area, shallow ground water can discharge to streams or migrate to deeper aquifers typically used for drinking-water purposes. As a result, nitrate in shallow ground water has the potential to affect the quality of those resources as well.

Elevated concentrations of nitrate in drinking water have been associated with adverse health effects, especially for newborns. Infants younger than 6 months old who are fed formula made from water containing nitrate may develop "blue baby" syndrome (methemoglobinemia). In this condition, blood loses its ability to transport oxygen to tissues in the body, which potentially is fatal. For this reason, the U.S. Environmental Protection Agency established the drinking-water standard of 10 mg/L nitrate as nitrogen. Additionally, nitrate concentrations of 2–4 mg/L have been associated with adverse health effects. Long-term (many years) exposure to nitrate in community water supplies has possible links to bladder and ovarian cancer (Weyer and others, 2001) and non-Hodgkins lymphoma (Ward and others, 1996).

Nitrogen input is one influence on nitrate contamination of shallow ground water

The sources of nitrogen in watersheds are primarily inorganic fertilizer, animal manure, and airborne emissions from utilities, factories, and automobiles. In areas of intensive agriculture, fertilizer usually is the predominant source of nitrogen. Animal manure and atmospheric deposition account for smaller amounts of nitrogen contributions nationally than commercial fertilizer, but are significant secondary sources of nitrogen in certain regions. Septic systems can be important local sources of nitrogen, especially in rural or residential areas. Lawn fertilizers and pet wastes are sources of nitrogen in urban areas. Natural sources of nitrogen include exchangeable ammonium in certain geologic deposits, nitrogen fixation (bacterial conversion of nitrogen in the air to organic nitrogen), and plant matter and other organic materials.

Water-quality studies indicate that high fertilizer application and irrigation offer a high potential for nitrate to move down to the water table. Increasing amounts of nitrate applied to the land surface, however, do not necessarily result in uniform increases in nitrate concentrations in shallow ground water. In some areas with permeable soils where nitrate is readily transmitted to the water table, nitrate levels may be higher than expected even though nitrate input is relatively low. In other areas, because conditions restrict nitrate from moving to the water table, nitrate levels may be lower than expected despite relatively high input.

Aquifer susceptibility to nitrate contamination is related to many hydrogeologic characteristics that determine the behavior of nitrate in the landscape

Nitrate can be carried through soils to the water table by percolating rainfall, snowmelt, and irrigation water. Soil drainage characteristics influence how fast nitrate travels through the soil and whether nitrate reaches the ground water. Well-drained soils, such as coarse-textured sands, transmit water and nitrate rapidly to the water table. Poorly drained soils, such as fine-grained clays, restrict water from infiltrating to the water table. Poorly drained soils also lack oxygen, a condition that promotes conversion of nitrate to nitrogen gas (denitrification) and limits conversion of dissolved ammonia to nitrate (nitrification). In general, unconsolidated sand and gravel aquifers are porous and allow rapid movement of water, making them more susceptible to contamination from nitrate, whereas relatively impermeable layers of rock, silt or clay inhibit infiltration. Fractured rocks and karst also provide conduits for water and nitrate to travel to shallow ground water. The pathway between surface runoff and ground water in some areas with waterlogged soils is often short-circuited by ditches and drains. These ditches and drains can intercept shallow ground water containing dissolved nitrate and divert the ground water to nearby streams.

Fundamentals of designing a model of nitrate contamination of shallow ground water

A model is a simplified representation of complex real-world processes. Statistical models describe the processes in terms of a set of selected explanatory variables, and attempt to predict what will happen when systematically changing the values of the explanatory variables. The relation of the explanatory variables to the predicted outcome is expressed as a mathematical equation. The predicted outcome is calculated from the explanatory variables that go into the mathematical expression.

Logistic regression is a statistical method that uses one or more independent explanatory variables to explain a yes/no outcome. For example, in this model, the outcome could be "yes, nitrate concentration is more than 4 mg/L" or "no, nitrate concentration is 4 mg/L or less." The modeled response is the probability of an outcome rather than a specific concentration.

The following general steps used in building a statistical model are illustrated by specific examples from the model of potential nitrate contamination of shallow ground water:

1. Define the underlying assumptions concerning the real-world processes that the model is intended to represent. Identify the possible explanatory variables and envision their effects on the result of interest. Assemble data sets describing the explanatory variables so that the variables can be quantified. In this case:

   ■ Nitrate contamination of shallow ground water depends on many factors concerning nitrogen input and aquifer susceptibility.

   ■ The candidate explanatory variables were compiled as national data sets to the extent possible. The availability of national data sets had to be considered, because some variables could not be mapped at the national scale.

   ■ Thirteen candidate explanatory variables describing nitrogen input and aquifer susceptibility were identified as possible influences on nitrate contamination of shallow ground water.

2. Screen the candidate explanatory variables to select which ones best explain the data. Modify or delete the variables that are not significant in the model. Write an equation that relates the selected variables to the desired outcome, in this case, whether nitrate is greater or less than 4 mg/L.

   ■ Thirteen candidate explanatory variables representing nitrogen input and aquifer susceptibility were evaluated using logistic regression to determine their influence on nitrate contamination of shallow ground water on a national level.

   ■ The list was narrowed to six variables that had a significant influence on nitrate contamination of shallow ground water. Variables that did not have a significant effect at the national scale may affect nitrate leaching locally.

   ■ The final six variables found to have the most influence on nitrate contamination of shallow ground water are fertilizer applications, agricultural land use, and population density *(nitrogen input)*, and soil drainage, water-table depth, and sand and gravel aquifers *(aquifer susceptibility)*.

3. Calibrate the model using measured data.

   ■ The model was calibrated using water-quality data collected from 1,280 wells in 20 NAWQA study areas sampled during 1992–95.

   ■ The model correctly predicted the nitrate status in 68 percent of the wells used for calibration.

4. Validate the model by checking how well the model predictions match actual measurements for wells not included in the model calibration. In this case:

   ■ The model was validated using water-quality data collected from 736 wells in 16 other NAWQA study areas sampled during 1996–99.

   ■ The probabilities of nitrate contamination predicted by the model are reasonably well correlated to the probabilities observed for the validation data. The model correctly predicted the nitrate status in 75 percent of the wells used for validation.

5. Use the model to attempt to predict results in areas not observed directly.

   ■ The model was used to predict the probability of nitrate contamination of shallow ground water in unsampled areas of the United States. *(See probability map on reverse side.)*

Candidate explanatory variables evaluated for model

Variables representing nitrogen input

➤ (1) Nitrogen fertilizer applications
➤ (2) Total nitrogen (fertilizer + manure + atmospheric deposition) applications
➤ (3) Percentage of agricultural land use
➤ (4) 1990 population density

Variables representing aquifer susceptibility

(5) Certain well-drained soils
➤ (6) Percentage of all well-drained soils
(7) Percent organic matter in soils
➤ (8) Depth to seasonally high water table
(9) Presence or absence of rock fracture
(10) Artificially drained soils
(11) Woodland-to-cropland ratio
(12) Sampling depth
(13) Mean annual precipitation, 1961–90

➤ Indicates candidate variable was selected for further analysis.

Explanatory variables selected for model

Variables representing nitrogen input

(1) Nitrogen fertilizer applications
(2) Percentage of agricultural land use
(3) 1990 population density

Variables representing aquifer susceptibility

(4) Percentage of well-drained soils
(5) Depth to seasonally high water table
(6) Presence or absence of sand and gravel aquifers
(The variable for sand and gravel aquifers replaced the variable for rock fracture.)

The set of explanatory variables evolved as the model of probability of nitrate contamination of shallow ground water was refined.

NAWQA study unit sampled during 1992–99
● Well used for calibration
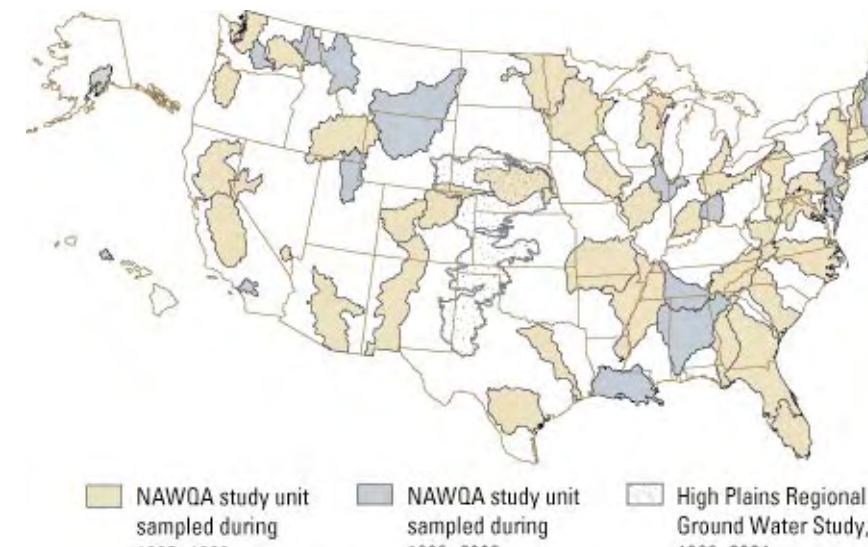● Well used for validation
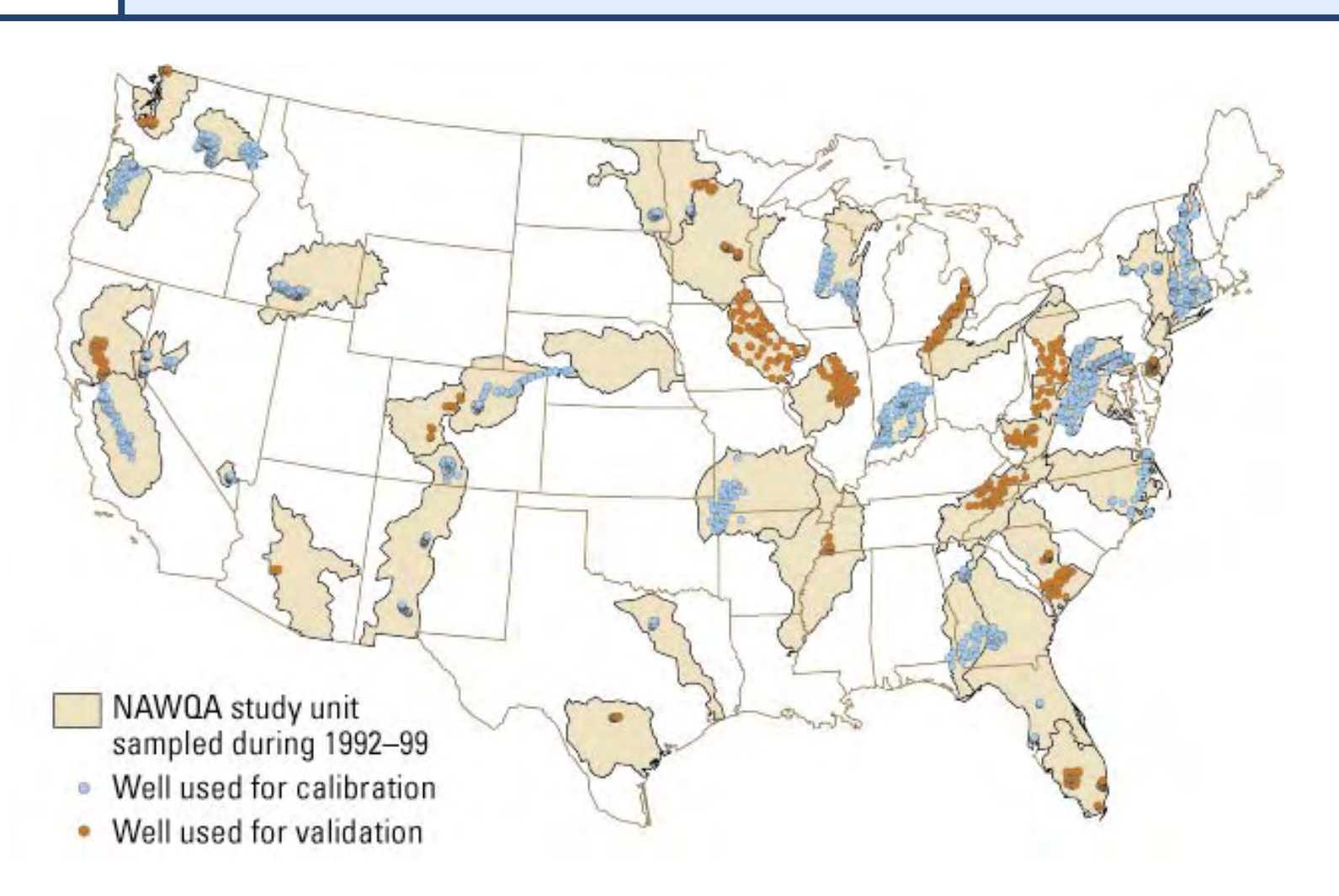
Suggested Reading

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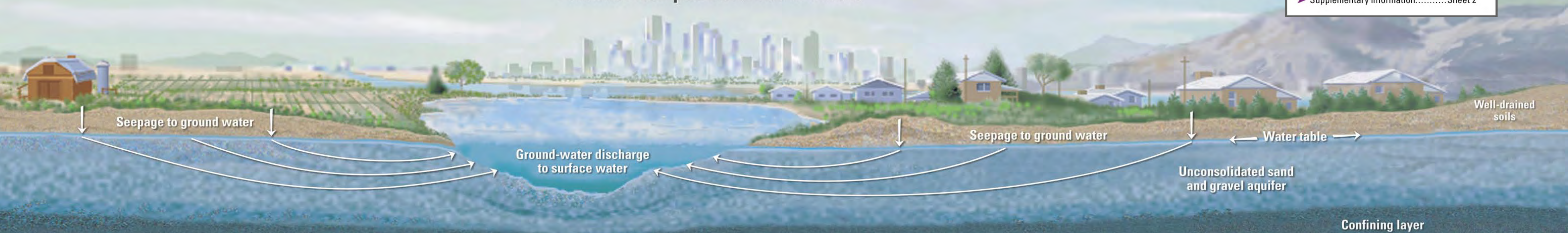
National Water-Quality Assessment (NAWQA) Program

NAWQA is a nationwide assessment of water quality. The NAWQA Program seeks to improve scientific and public understanding of water quality in the Nation's major river basins and ground-water systems. The goals of NAWQA are to assess the status and trends of national water quality and to understand the factors that affect it. NAWQA assessments support the investigation of local issues and trends, while providing a firm foundation for understanding water quality at regional and national scales. NAWQA assessments of major river basins and aquifers (called NAWQA "study units") adhere to a national design and nationally consistent sampling and analytical methods. Collectively, the 51 study units cover about one-half of the land area of the United States and include water resources that are available to more than 60 percent of the Nation's population. Land-use studies examine the water quality of shallow, recently recharged ground water underlying a relatively uniform land-use setting, such as cropland or residential. Each study collects data from a network of about 30 wells. The information provided by NAWQA supports national, regional, State, and local decision-making and guides policy formation for water-quality management.

More detailed and technical information supporting this document is available in the Environmental Science & Technology article "Probability of nitrate contamination of recently recharged groundwaters in the conterminous United States," by Nolan and others (2002), which is available online at: *http://water.usgs.gov/nawqa/nutrients/pubs/est_v36_no10/*. The probabilities of nitrate contamination in shallow ground water shown in the map (on reverse side) are available in a geographic information system (GIS) format at: *http://water.usgs.gov/lookup/getspatial?gwrisk*.

NAWQA study unit sampled during 1992-1999
NAWQA study unit sampled during 1999-2003
High Plains Regional Ground Water Study, 1999-2004

Potential Non-point Sources of Nitrate

Seepage to ground water
Ground-water discharge to surface water
Seepage to ground water
Water table
Well-drained soils
Unconsolidated sand and gravel aquifer
Confining layer

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