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Application of Health-Based Screening Levels to Ground-Water Quality Data in a State-Scale Pilot Effort

Scientific Investigations Report 2004-5174

Prepared in cooperation with the New Jersey Department of Environmental Protection
and Oregon Health & Science University

U.S. Department of the Interior
U.S. Geological Survey

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By Patricia L. Toccalino, Julia E. Norman, Robyn H. Phillips, Leon J. Kauffman, Paul E. Stackelberg, Lisa H. Nowell, Sandra J. Krietzman, and Gloria B. Post

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U.S. Department of the Interior
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U.S. Geological Survey, Reston, Virginia: 2004
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Suggested citation:
Toccalino, P.L., Norman, J.E., Phillips, R.H., Kauffman, L.J., Stackelberg, P.E., Nowell, L.H., Krietzman, S.J., and Post, G.B., 2004, Application of health-based screening levels to ground-water quality data in a state-scale pilot effort: U.S. Geological Survey Scientific Investigations Report 2004-5174, 64 p.

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Conversion Factors, Abbreviations, and Acronyms

Multiply	By	To obtain
foot (ft)	0.3048	meter
gallon per day (gal/d)	0.003785	cubic meter per day
square mile (mi^2)	2.590	square kilometer
kilogram (kg)	2.205	pound avoirdupois
liter (L)	0.2642	gallon
micrograms per liter (µg/L)	1.0	parts per billion

<	less than
>	greater than or equal to
µg/L	micrograms per liter
BQ	Benchmark Quotient
BQmax	Ratio of maximum detected concentration to drinking-water benchmark
BQmed-det	Ratio of median of detected concentrations to drinking-water benchmark
BQmed-all	Ratio of median of all samples (including non-detections) to drinking-water benchmark
BQSiteMax	Maximum of BQ values for detected compounds in a given well
BQSiteSum	Sum of all BQ values for detected compounds in a given well
CASRN	Chemical Abstracts Service Registry Number
E	Estimated Concentration

GWQC	Ground Water Quality Criteria (New Jersey Department of Environmental Protection)
GWQS	Ground Water Quality Standards (New Jersey Department of Environmental Protection)
HBSL	Health-Based Screening Level
HEAST	Health Effects Assessment Summary Tables
HI	Hazard Index
HQ	Hazard Quotient
IRIS	Integrated Risk Information System (U.S. Environmental Protection Agency)
Lifetime HA	Lifetime Health Advisory
LINJ	Long Island – New Jersey
LRL	Laboratory Reporting Level
LT-MDL	Long-Term Method Detection Level
MCL	Maximum Contaminant Level
MRL	Minimum Reporting Level
MTBE	Methyl *tert*-butyl ether
NAWQA	National Water-Quality Assessment Program
NJDEP	New Jersey Department of Environmental Protection
NWQL	National Water Quality Laboratory
OHSU	Oregon Health & Science University
OPP	Office of Pesticide Programs (U.S. Environmental Protection Agency)
ORD	Office of Research and Development (U.S. Environmental Protection Agency)
OW	Office of Water (U.S. Environmental Protection Agency)
PCE	Tetrachloroethylene
PQL	Practical Quantitation Level
q_1^*	Cancer Potency Factor (see also SF)
RfD	Reference Dose
RSD	Risk-Specific Dose
SF	Slope Factor
SOC	Synthetic Organic Chemical
TCE	Trichloroethylene
USEPA	U.S. Environmental Protection Agency
USGS	U.S. Geological Survey
VOC	Volatile Organic Compound

Application of Health-Based Screening Levels to Ground-Water Quality Data in a State-Scale Pilot Effort

By Patricia L. Toccalino[1], Julia E. Norman[1], Robyn H. Phillips[1], Leon J. Kauffman[2], Paul E. Stackelberg[2], Lisa H. Nowell[3], Sandra J. Krietzman[4], and Gloria B. Post[4]

Abstract

A state-scale pilot effort was conducted to evaluate a Health-Based Screening Level (HBSL) approach developed for communicating findings from the U.S. Geological Survey (USGS) National Water-Quality Assessment Program in a human-health context. Many aquifers sampled by USGS are used as drinking-water sources, and water-quality conditions historically have been assessed by comparing measured contaminant concentrations to established drinking-water standards and guidelines. Because drinking-water standards and guidelines do not exist for many analyzed contaminants, HBSL values were developed collaboratively by the USGS, U.S. Environmental Protection Agency (USEPA), New Jersey Department of Environmental Protection, and Oregon Health & Science University, using USEPA toxicity values and USEPA Office of Water methodologies. The main objective of this report is to demonstrate the use of HBSL approach as a tool for communicating water-quality data in a human-health context by conducting a retrospective analysis of ground-water quality data from New Jersey. Another important objective is to provide guidance on the use and interpretation of HBSL values and other human-health benchmarks in the analyses of water-quality data in a human-health context.

Ground-water samples collected during 1996-98 from 30 public-supply, 82 domestic, and 108 monitoring wells were analyzed for 97 pesticides and 85 volatile organic compounds (VOCs). The occurrence of individual pesticides and VOCs was evaluated in a human-health context by calculating Benchmark Quotients (BQs), defined as ratios of measured concentrations of regulated compounds (that is, compounds with Federal or state drinking-water standards) to Maximum Contaminant Level (MCL) values and ratios of measured concentrations of unregulated compounds to HBSL values. Contaminants were identified as being of potential human-health concern if maximum detected concentrations were within a factor of 10 of the associated MCL or HBSL (that is, maximum BQ value (BQmax) greater than or equal to 0.1) in any well type (public supply, domestic, monitoring). Most (57 of 77) pesticides and VOCs with human-health benchmarks were detected at concentrations well below these levels (BQmax less than 0.1) for all three well types; however, BQmax values ranged from 0.1 to 3,000 for 6 pesticides and 14 VOCs. Of these 20 contaminants, one pesticide (dieldrin) and three VOCs (1,2-dibromoethane, tetrachloroethylene, and trichloroethylene) both (1) were measured at concentrations that met or exceeded MCL or HBSL values, and (2) were detected in more than 10 percent of samples collected from raw ground water used as sources of drinking water (public-supply and (or) domestic wells) and, therefore, are particularly relevant to human health.

The occurrence of multiple pesticides and VOCs in individual wells also was evaluated in a human-health context because at least 53 different contaminants were detected in each of the three well types. To assess the relative human-health importance of the occurrence of multiple contaminants in different wells, the BQ values for all contaminants in a given well were summed. The median ratio of the maximum BQ to the sum of all BQ values for each well ranged from 0.83 to 0.93 for all well types, indicating that the maximum BQ makes up the majority of the sum for most wells. Maximum and summed BQ values were statistically greater for individual public-supply wells than for individual domestic and monitoring wells.

The HBSL approach is an effective tool for placing water-quality data in a human-health context. For 79 of the 182 compounds analyzed in this study, no USEPA drinking-water standards or guidelines exist, but new HBSL values were calculated for 39 of these 79 compounds. The new HBSL values increased the number of detected pesticides and VOCs with human-health benchmarks from 65 to 77 (of 97 detected compounds), thereby expanding the basis for interpreting contaminant-occurrence data in a human-health context.

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Introduction

An interagency pilot effort was conducted to test an approach for communicating water-quality findings in a human-health context in state- and local-scale reports. There were two stages to this pilot effort. In the first stage, consensus was reached on the development of **Health-Based Screening Level (HBSL)**[1] values for unregulated contaminants, that is, those for which **drinking-water standards** have not been established. The U.S. Geological Survey (USGS) conducted a study, in cooperation with the U.S. Environmental Protection Agency (USEPA), the New Jersey Department of Environmental Protection (NJDEP), and Oregon Health & Science University (OHSU), to collaboratively develop the HBSL approach for application to state- and local-scale water-quality assessments. The systematic procedures used to develop HBSL values are described in Toccalino and others (2003). The second stage of the pilot effort, the subject of this report, consists of the application of HBSL values as tools for describing water-quality data in a human-health context in a state-scale water-quality assessment.

The ground-water data described in this report were collected for the Long Island-New Jersey (LINJ) Coastal Drainages Study Unit (Ayers and others, 2000) as part of the USGS National Water-Quality Assessment (NAWQA) Program. Work in the LINJ Study Unit, which includes some of the most heavily urbanized and populated areas in the United States, began in 1994 (Ayers and others, 2000). The HBSL approach was applied to ground-water quality data collected from 220 wells in the LINJ Study Unit during 1996-98. These ground-water quality data have been presented previously in numerous publications (Ayers and others, 2000; Clawges and others, 1999; Kauffman and others, 2001; Stackelberg and others, 1997, 2000, and 2001), but the potential human-health implications of these water-quality data have not been interpreted previously using HBSL values.

Purpose and Scope

The objective of this report is two-fold. A major objective is to demonstrate the HBSL approach as a tool for communicating water-quality data in a human-health context by performing a retrospective analysis of ground-water quality data collected as part of the USGS NAWQA Program in New Jersey. One ground-water sample was collected from each public-supply, domestic, and monitoring well in the study unit during 1996-98. Samples were analyzed for a total of 97 pesticides and 85 volatile organic compounds (VOCs), and measured concentrations were compared to USEPA and New Jersey Maximum Contaminant Level (MCL) values or HBSL values. The use of HBSL values allows for an extended interpretation of the potential human-health implications of water-quality data because HBSL values exist for some compounds that previously had no **human-health benchmarks**. Another important objective of this report is to provide guidance on the use and interpretation of HBSL values and other human-health benchmarks in the analyses of water-quality data in a human-health context by considering factors such as the magnitude of detected concentrations relative to human-health benchmarks, detection frequency, well type, and use of water.

The scope of this pilot effort is confined to the consideration of ground-water data because ground water is the principal drinking-water source in the study unit area (Stackelberg and others, 1997). This pilot effort primarily examines the occurrence of individual (single) chemicals detected in ground-water samples in a human-health context, although initial efforts also are undertaken to evaluate the relative occurrence of multiple contaminants in individual wells in a human-health context because numerous contaminants were detected in each well type. Additionally, this pilot effort does not attempt to provide estimates of the numbers of people potentially exposed to the ground-water resources in the study unit, which is beyond the scope of this report, although factors that affect potential exposure, such as well type and the physicochemical properties of contaminants, are discussed.

Need for and History of the Human-Health Pilot Effort

In 1991, the USGS began the NAWQA Program to (1) provide a consistent description of current water-quality conditions for a large part of the Nation's water resources; (2) define any long-term trends in water quality; and (3) identify, describe, and explain, to the extent possible, the major natural and human factors that affect observed water-quality conditions and trends (Leahy, 1990). The USGS has been asked with increasing frequency about the public-health implications of the NAWQA findings. The NAWQA Program originally was designed to characterize the Nation's water resources and was not designed to answer questions about the potential safety of these water resources for drinking-water use. Nonetheless, if interpreted carefully, NAWQA data on ground-water quality can provide valuable information to state agencies, the USEPA, and others interested in drinking-water quality.

To date, NAWQA has assessed water-quality conditions using two approaches. The first approach ranks water-quality conditions at individual surface-water sites and among networks of ground-water wells within a study unit in relation to conditions at surface-water sites and ground-water networks, respectively, in other study units. The second approach compares measured contaminant concentrations against established drinking-water standards and guidelines for the protection of human health (Gilliom and others, 1998). The first approach provides no information on whether the contaminant-concentration levels detected are of potential concern to human health, and the second approach is limited by the fact that drinking-water standards and guidelines do not exist for many of the

[1]Words in bold are defined in the glossary at the end of the report.

contaminants analyzed in NAWQA studies. Therefore, the USGS has undertaken this HBSL initiative to more comprehensively evaluate its water-quality findings in a human-health context.

Over a 3-year period beginning in October 1998, a consensus HBSL approach was developed collaboratively by the USGS, USEPA, NJDEP, and OHSU. During this time, multiple procedures for assessing water-quality data in a human-health context were considered for this pilot effort, including procedures used by different programs and offices within USEPA (including Office of Water (OW), Office of Pesticide Programs (OPP), Office of Research and Development (ORD), and Office of Solid Waste and Emergency Response). The consensus decision was to use USEPA OW methodologies in developing the HBSL approach because this pilot effort addresses groundwater resources that are, or contribute to, drinking-water resources. The decision also was made to begin by applying the HBSL approach to a state-scale pilot effort. The LINJ Study Unit was selected as an appropriate pilot study for state-scale analyses because water-quality data were available from multiple well types and hydrogeologic settings. A complete history of this pilot effort, as well as the HBSL approach and methods, is described in Toccalino and others (2003). The HBSL approach is summarized in the following section.

Development and Use of Health-Based Screening Level Values

Health-Based Screening Level values are defined as estimates of benchmark concentrations (for noncarcinogens) or concentration ranges (for carcinogens) of contaminants in water that (1) may be of potential human-health concern; (2) can be used as threshold values against which measured concentrations of contaminants in ambient water samples can be compared; and (3) are consistent with USEPA OW methodologies for setting drinking-water **Lifetime Health Advisory** (Lifetime HA) and **Risk-Specific Dose** (RSD) values (Toccalino and others, 2003; U.S. Environmental Protection Agency, 1988, 1993). HBSL values are not drinking-water standards, nor are they USEPA or NJDEP guideline values. HBSL values are useful thresholds, however, for determining when measured concentrations meet or exceed concentrations relevant to human health. HBSL values are developed by using USEPA OW methodologies and USEPA toxicity values, so they are as comparable as possible to USEPA **drinking-water guideline** values (that is, Lifetime HA and RSD values). As used in this report, **new HBSL** values refer to HBSL values calculated for unregulated contaminants that (1) have no existing USEPA drinking-water guideline values or (2) have more recent USEPA toxicity data than that used to calculate existing USEPA drinking-water guideline values, resulting in different benchmark values.

The USGS, USEPA, NJDEP, and OHSU participants in this pilot effort came to a consensus agreement to pursue the following two-tiered, screening-level-based methodology for placing NAWQA water-quality data in a human-health context for state- and local-scale analyses and reports (Toccalino and others, 2003):

- Tier 1: For **regulated compounds** (compounds for which Federal and (or) state drinking-water standards have been established), compare measured contaminant-concentration data with USEPA MCL values and applicable state drinking-water standards.
- Tier 2: For **unregulated compounds** (compounds for which Federal and (or) state drinking-water standards have not been established), compare measured contaminant-concentration data with HBSL values developed using USEPA OW methodologies (U.S. Environmental Protection Agency, 1988 and 1993) and USEPA toxicity data.

This two-tiered approach for state- and local-scale analyses entails listing regulated compounds separately from unregulated compounds. For regulated compounds, measured concentration data will continue to be compared with Federal and (or) state drinking-water standard values as has been done historically. Standard values are threshold values that are legally enforceable by Federal or state government agencies. For purposes of comparison with contaminant concentrations measured by the USGS in raw water, these standards will not be used as regulatory values; rather, these standards will be used as benchmarks that provide some information about the potential health effects if the sampled water resources were to be consumed over a lifetime by the average adult. HBSL values will be used only for compounds for which no drinking-water standards have been established by USEPA or NJDEP (that is, unregulated compounds). Other states may have a different number of compounds with drinking-water standards than New Jersey; therefore, the number of compounds for which it is appropriate to apply HBSL values will vary from state to state.

HBSL values were developed for unregulated compounds by using USEPA OW methodologies to calculate Lifetime HA and RSD values (U.S. Environmental Protection Agency, 1988 and 1993) and toxicity values published by the USEPA Integrated Risk Information System (IRIS), OW, OPP, and in the Health Effects Assessment Summary Tables (HEAST). A detailed description of the methodologies used to develop HBSL values is presented in Toccalino and others (2003).

When MCL values (Tier 1) or HBSL values (Tier 2) are used as benchmarks for communicating water-quality data in a human-health context, there are important caveats to consider. Exceedance of MCL or HBSL values does not necessarily mean that people who potentially consume the water are adversely affected because (1) the USEPA OW models used to develop these benchmark values are intentionally conservative (protective) and include safety factors; (2) the models assume lifetime exposure to these concentrations, whereas the concentrations of contaminants may change seasonally or over time; and (3) the raw water resources from some well types typically sampled may be treated prior to consumption, and contaminant concentrations may be reduced substantially by treatment methods (Toccalino and others, 2003). Not all well types

receive treatment, however, and the treatment methods may not be designed to remove specific contaminants from the water resources.

Description of Study Area

The LINJ Coastal Drainages Study Unit includes all of New Jersey, except for those areas that drain to the Delaware and Hudson River Basins, and all of Long Island (fig. 1) (Ayers and others, 2000). The ground-water data described in this report were collected in New Jersey, with the exception of data from three samples that were collected in New York State. The extent of the sampled area also includes the Glassboro study area, a 380-square-mile section of southern New Jersey. Part of the Glassboro study area falls outside of the LINJ Study Unit boundary (fig. 1).

The study area includes three ground-water sampling regions in New Jersey (fig. 1). The Kirkwood-Cohansey aquifer system in southern New Jersey consists of unconsolidated sedimentary deposits (sands and gravels) (Ayers and others, 2000), whereas aquifers in the New England and Piedmont Physiographic Provinces in northern New Jersey consist of fractured bedrock (Clawges and others, 1999). The chemical quality of ground water in these three aquifers is of concern because they are important sources of drinking water (Ayers and others, 2000). All three aquifers are vulnerable to contamination introduced at or near the land surface. The vulnerability of the Kirkwood-Cohansey aquifer system results from the highly permeable unconsolidated sands and gravels composing the aquifer system (Stackelberg and others, 1997) and the shallow depth to ground water; the average depth to ground water in the Glassboro study area is about 15 feet below ground surface (Stackelberg and others, 2000). The vulnerability of the bedrock aquifers in the New England and Piedmont Physiographic Provinces varies depending on soil and rock type and the degree of fracturing of the rock (Clawges and others, 1999); fractures can serve as conduits to deeper parts of the aquifers. The New England Physiographic Province is equivalent to the Highlands, which is the physiographic term used by NJDEP.

The chemical quality of ground water in the Glassboro area, which is part of the Kirkwood-Cohansey aquifer system, is of particular concern because this is a fast-growing region of New Jersey and because ground water provides most of the public and domestic supply in the area (Stackelberg and others, 1997). As a result of NJDEP-mandated restrictions on withdrawals from deeper confined aquifers (New Jersey Department of Environmental Protection, 1996), the surficial Kirkwood-Cohansey aquifer system has experienced increased withdrawals to meet growing water-supply demands in the area (Stackelberg and others, 1997). About half of the water withdrawn from the Kirkwood-Cohansey aquifer system in the Glassboro area is for public- and domestic-water supplies. The remaining half is withdrawn for industrial and irrigation purposes (Kauffman and others, 2001).

Well Networks

Raw (that is, untreated) ground-water samples were collected from three different well types: public-supply wells (30 samples), domestic wells (82 samples), and monitoring wells (108 samples). Water-quality data from each of these well types contributes different information towards the objective of communicating contaminant-occurrence data in a human-health context. Except for domestic-well samples, which were collected from three major sampling regions throughout the LINJ Study Unit (fig. 1), the remaining ground-water samples discussed in this report were collected from the Glassboro study area.

Design of Public-Supply Well Network

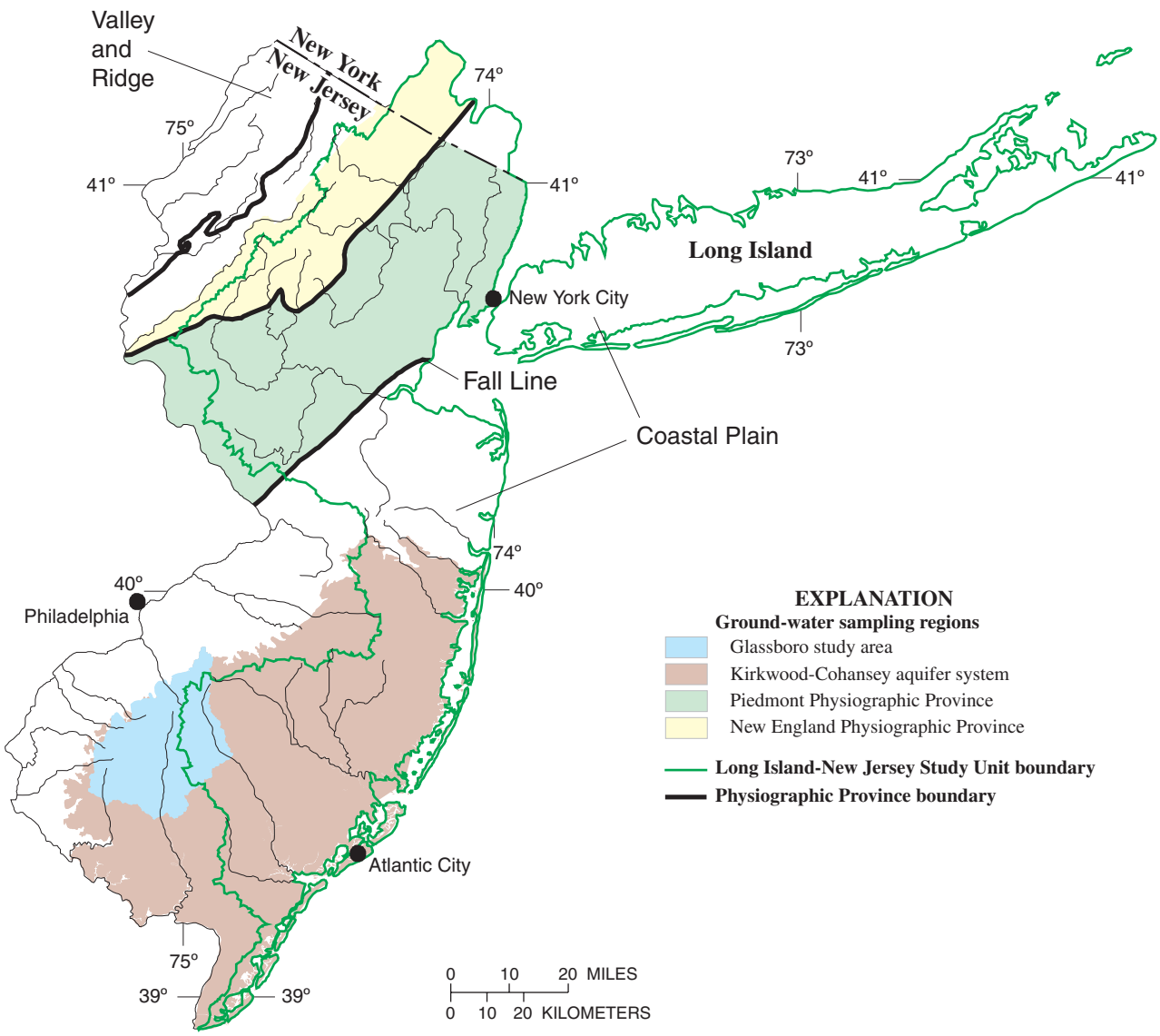
Thirty public-supply wells (fig. 2a) in the Glassboro study area were sampled once either in 1997 or 1998 to determine the chemical quality of ground water in the part of the Kirkwood-Cohansey aquifer system used for public supply. Data from these wells also were used in conjunction with data from the land-use monitoring wells and a ground-water model to better understand how contaminants enter and move through the aquifer to water-supply wells and streams (Kauffman and others, 2001). Public-supply wells usually are in urban areas.

The public-supply wells are screened over intervals ranging from 15 to 47 feet, and have well depths ranging from 71 to 180 feet below ground surface. The average pumping rate during 1992-96 was about 270,000 gallons per day (unpublished data on file at USGS New Jersey District office, West Trenton, N.J.). Because public-supply wells withdraw large volumes of water, they have correspondingly large contributing areas that generally encompass multiple land uses (Stackelberg and others, 2001).

If water from a public-water system exceeds USEPA or New Jersey MCL values, the supplier of that water is required to eliminate the problem by changing to or adding another water source or by improving water treatment within 1 year (New Jersey Department of Environmental Protection, 2000). The ground-water samples in this study were collected prior to any treatment and do not represent finished drinking-water samples. As a result, any measured contaminant concentration in the raw water resources that exceeds Federal or state MCL values does not indicate a violation of drinking-water standards, and no corrective action is required (although the NJDEP generally is notified in these cases).

Design of Domestic-Well Networks

Ground-water samples were collected from 82 domestic (household) wells in New Jersey to characterize water quality that is representative of three sampling regions (fig. 2b). Ground-water samples were collected from domestic-well networks located in an unconsolidated sediment aquifer

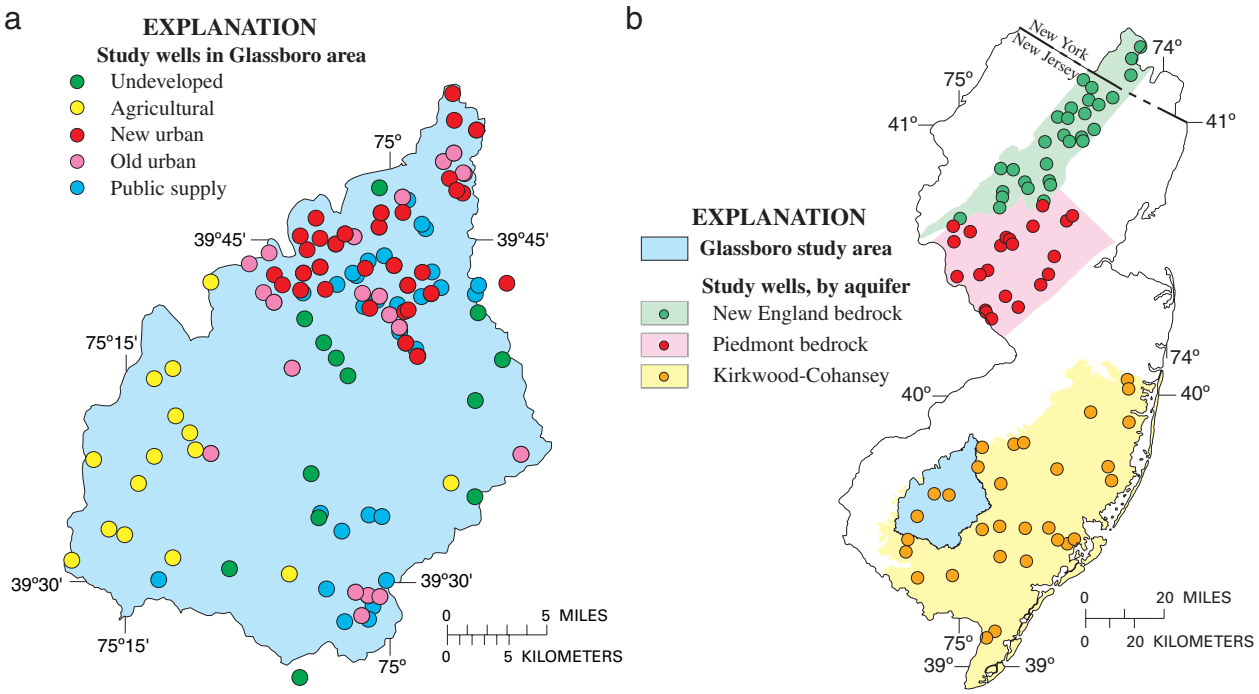


Base from U.S. Geological Survey digital data, 1:200,000, 1985
Universal Transverse Mercator projection, Zone 18
North American Datum of 1983

Figure 1. Ground-water sampling regions in the Long Island-New Jersey Coastal Drainages Study Unit and the Glassboro study area (modified from Ayers, 1994).

(30 domestic wells in the Kirkwood-Cohansey aquifer system) and in fractured bedrock aquifers (30 domestic wells in the New England Physiographic Province and 22 domestic wells in the Piedmont Physiographic Province). Each of the 82 domestic wells was sampled once. Wells in the New England and Piedmont Physiographic Provinces were sampled in 1997, and wells in the Kirkwood-Cohansey aquifer system were sampled in 1998 (Ayers and others, 2000).

Domestic wells are private sources of water supply primarily found in rural or agricultural settings rather than dense urban areas. Domestic wells tapping the unconsolidated sediments of the Kirkwood-Cohansey aquifer system are screened over 5- to 10-foot-long intervals to depths ranging from 38 to 175 feet below ground surface. In contrast, domestic wells in the fractured bedrock aquifers have open intervals over much of their length. In the New England Physiographic Province, the domestic wells are open over intervals ranging from 6 to 263 feet, and to depths ranging from 150 to 300 feet below ground surface. In the Piedmont Physiographic Province, domestic wells are open over intervals ranging from 90 to 200 feet, and to depths of 125 to 250 feet below ground surface. Domestic wells pump an average of 82 gallons of water per day per person, equivalent to approximately 320 gallons per day for a four-person household (Nawyn, 1998).



Base from U.S. Geological Survey digital data, 1:200,000, 1985
Universal Transverse Mercator projection, Zone 18
North American Datum of 1983

Figure 2. Location of (a) public-supply and monitoring wells in the Glassboro study area of the Kirkwood-Cohansey aquifer system, New Jersey, and (b) domestic wells, by aquifer (sampling region), in the Long Island-New Jersey Coastal Drainages Study Unit (from Ayers and others, 2000).

Design of Monitoring-Well Networks

Ground-water samples were collected from a network of 108 monitoring wells in the rapidly urbanizing Glassboro study area (fig. 2a), including 78 shallow monitoring wells (about 10 feet below the water table) and 30 moderate-depth monitoring wells (about 40-50 feet below the water table). Monitoring-well data provide a great deal of information about contaminant sources, the environmental fate and transport of contaminants, and trends in contaminant concentrations over time. Ground water collected from monitoring wells also can be a source to, and a predictor of, contaminant concentrations in parts of the aquifer used for domestic and public supply at some later period of time (Stackelberg and others, 1997).

The 78 shallow monitoring wells were used to measure the effects of land use on shallow ground-water quality and to assess the chemical quality of recently recharged (shallow) ground water in the surficial Kirkwood-Cohansey aquifer system (fig. 2a) of southern New Jersey. Four land-use settings were investigated: agricultural areas (15 wells), areas of residential and commercial development less than 25 years old (30 new urban wells), areas of residential and commercial development more than 25 years old (20 old urban wells), and undeveloped areas (13 wells) (Ayers and others, 2000; Stackelberg and others, 1997). The undeveloped land uses primarily are forested areas and wetlands, but may contain small amounts of urban or agricultural land. Each of the 78 shallow monitoring wells was sampled once during September-December 1996.

Additionally, 30 ground-water samples were collected from a network of 30 moderate-depth monitoring wells in the Glassboro study area that are co-located with 30 shallow monitoring wells in urban land-use areas. Each of the moderate-depth monitoring wells was sampled once during fall 1997. Samples from these wells were collected in order to evaluate the quality of ground water recharged in urban areas 10 to 20 years ago (Stackelberg and others, 2000). The chemical quality of 10- to 20-year-old water is of concern because ground-water modeling results indicate that water withdrawn from the Kirkwood-Cohansey aquifer system for domestic and public supply is composed partly of water from this age interval. Additionally, the quality of this water resource is an indicator of the fate of contaminants known to be contributing to the contaminant load at the water table in areas of urban development (Stackelberg and others, 2000).

The shallow monitoring wells typically were screened over 2-foot-long intervals approximately 10 feet below the water table (Stackelberg and others, 1997). Shallow monitoring wells were sampled at depths near the water table (Ayers and

others, 2000) and, therefore, capture water flowing in paths that originate in relatively small areas at the land surface (Stackelberg and others, 2000). In contrast, the moderate-depth monitoring wells typically were screened over 2- to 2.5-foot-long intervals (Stackelberg and others, 2000), approximately 40 to 50 feet below the water table (Ayers and others, 2000). Well-screen depths were selected by using ground-water flow modeling tools developed by the USGS (Stackelberg and others, 2000). All monitoring wells were pumped only during sampling and at very low rates (generally less than 1 gallon per minute) for short periods of time (generally less than 1 hour).

Analytical Considerations for Ground-Water Quality Data

Several analytical considerations need to be accounted for when interpreting water-quality data in a human-health context. These considerations include reporting Minimum Reporting Level (MRL) values for detected contaminants, identifying estimated concentrations of confirmed detections, explaining how detection frequencies were calculated, and comparing MRL values to human-health benchmarks. These considerations are described further below.

Minimum Reporting Levels and Estimated Concentrations

Sampling and analytical methods used in this study allowed for the quantification of pesticide concentrations with MRL values ranging from 0.001 to 1.2 micrograms per liter (μg/L) and VOC concentrations with MRL values ranging from 0.026 to 9 μg/L in ground-water samples. The MRL is defined as the smallest measured concentration of a compound that may be reliably reported by using a given analytical method (Timme, 1995). MRL values can change over time and can vary for different analytes within the same analytical method. Protocols and procedures used for sample collection are described in Koterba and others (1995). Analytical methods for pesticides and VOCs are described in Zaugg and others (1995), Werner and others (1996), and Connor and others (1998). The USGS National Water Quality Laboratory (NWQL) has implemented a procedure for establishing a default "less than" reporting level, called the laboratory reporting level (LRL), which is calculated from the long-term method detection limit (LT-MDL) (Oblinger Childress and others, 1999). In this report, MRL values are used because LRL and LT-MDL values did not come into use by the NWQL until 1999 (that is, after the data used in this report were generated).

The NWQL reports non-detections as less than (<) the MRL values and assigns E codes to estimated concentrations of confirmed detections of pesticides and VOCs that are less than the MRL (Oblinger Childress and others, 1999). A variety of conditions can justify evoking the E code, including results that were extrapolated beyond the calibration range used in the analytical method and matrix interferences in the sample (Kolpin, 2001; Oblinger Childress and others, 1999). All E-coded data are believed to be reliable detections but with greater than average uncertainty in quantification (U.S. Geological Survey, 1999). For most data analysis applications, E codes can be ignored because the qualitative difference in reliability is not substantial. If attention is placed on individual measured concentration values, then E-coded values are considered to be estimates only. All estimated concentrations are included in the calculation of detection frequencies and are presented in the figures and tables in this report.

Interpreting Detection Frequencies

Each of the 220 wells considered in this study were sampled once. The detection frequencies (that is, the percentage of samples with detections) in this report are given for all detections to provide a measure of how often a compound was detected in samples from a given well type. Detection frequencies tend to vary with the sensitivity of the analytical method used; if the MRL is lowered for a given compound, the detection frequency for that compound will tend to increase because lower concentrations of that compound can be detected. Therefore, the detection frequencies reported here are not directly comparable among compounds because the MRL varies between compounds (Kolpin, 2001), and sometimes for the same chemical over time as a result of changes in the analytical method or sample matrix effects. To aid in comparisons between compounds, the most common MRLs for each detected pesticide and VOC are included in this report.

A method commonly used by NAWQA to compare detection frequencies among compounds is to censor data to a common reporting level. The use of a common reporting level (or detection threshold) facilitates comparisons among compounds by bringing most of the data to a common reference point. Adjustments of this type are used to address questions such as "Is compound x detected more frequently than compound y?" (Kolpin, 2001). The data presented in this report are not censored to a common reporting level, however, because the primary focus of this report is to communicate water-quality results in a human-health context. Human-health benchmark concentrations such as HBSL and Ground Water Quality Criteria (GWQC) values are developed using toxicity data without consideration of analytical detection limits. Therefore, some HBSL values may be close to, or occasionally less than, MRL values, and censoring data to a common (typically higher) reporting level could lead to a loss of data that are relevant to human health. Censored data from LINJ studies that allow for comparison of detection frequencies between different compounds are available in previous publications (Ayers and others, 2000; Stackelberg and others, 2000).

Minimum Reporting Levels Compared to Human-Health Benchmarks

In order to ensure that the analytical methods are adequate to detect concentrations of potential human-health concern, the analytical MRL must be less than the human-health benchmark value. Fortunately, of the 87 pesticides and 55 VOCs analyzed in this study that have human-health benchmarks, 76 pesticides (87 percent) and 45 VOCs (82 percent) were reported with MRLs at least 10-fold less than the MCL or HBSL. This is a result of the low MRLs that can be achieved with USGS analytical methods.

Only five compounds (one pesticide and four VOCs) analyzed in ground-water samples from the LINJ Study Unit were reported with MRLs greater than their human-health benchmarks (MCL for regulated compounds and HBSL for unregulated compounds) (table 1). Two of the five compounds are regulated (1,2-dibromo-3-chloropropane and 1,2-dibromoethane), and three of the compounds are unregulated (aldrin, acrylonitrile, and methyl acrylonitrile). Only 1,2-dibromo-3-chloropropane and 1,2-dibromoethane were detected in ground-water samples collected from the LINJ Study Unit (table 1). The MRL for 1,2-dibromo-3-chloropropane (0.214 µg/L) is slightly greater than its MCL (0.2 µg/L), and the MRL for 1,2-dibromoethane (0.036 µg/L) is somewhat less than its MCL (0.05 µg/L) in most well types, although the MRLs for both compounds are approximately two-fold greater than their MCLs in shallow monitoring-well samples (table 1). Uncertainty in quantitation increases as detected concentrations approach the MRL. Benchmark exceedances for compounds with benchmarks below or near their respective MRL values also have greater uncertainty than for compounds with benchmarks greater than their MRL values.

Guidance for Interpreting Water-Quality Data in a Human-Health Context

An important objective of this report is to provide guidance on the use and interpretation of HBSL values and other human-health benchmarks in the analyses of water-quality data in a human-health context. This guidance is intended primarily for USGS personnel conducting state- or local-scale water-quality studies; however, it can also be applied more generally by other agencies or organizations to facilitate the interpretation of water-quality data in a human-health context. Effective use of human-health benchmarks in water-quality assessments requires an understanding of what the individual benchmarks mean, as well as information about the specific hydrologic system being studied. Three general steps are presented here for interpreting water-quality data in a human-health context. First, all applicable human-health benchmarks for detected contaminants are compiled and compared with measured concentrations. Second, contaminants of potential human-health concern are identified by assessing the differential between measured concentrations and human-health benchmarks. Lastly, the

Table 1. Pesticides and VOCs that have Minimum Reporting Levels that exceed human-health benchmarks in ground-water samples from the Long Island-New Jersey Study Unit.

[VOC, volatile organic compound; CASRN, Chemical Abstracts Service Registry Number; MRL, Minimum Reporting Level; µg/L, micrograms per liter; %, percent; SMW, shallow monitoring well; HBSL, Health-Based Screening Level; PSW, public-supply well; DW, domestic well; MDMW, moderate-depth monitoring well; MCL, Maximum Contaminant Level]

Compound	CASRN	MRL in µg/L (well type)	Human-health benchmark in µg/L (benchmark type)	Detection frequency (%)
		Pesticides		
Aldrin	309-00-2	0.01 (SMW)	0.002 to 0.2 (HBSL range)	Not detected
		VOCs		
Acrylonitrile	107-13-1	1.23 (PSW, DW, MDMW); 2 (SMW)	0.06 to 6 (HBSL range)	Not detected in any well type
1,2-Dibromo-3-chloropropane	96-12-8	0.214 (PSW, DW, MDMW); 0.5 (SMW)	0.2 (MCL)	1.2 in DW only
1,2-Dibromoethane	106-93-4	0.036 (PSW, DW, MDMW); 0.1 (SMW)	.05 (MCL)	13.3 in PSW only
Methyl acrylonitrile	126-98-7	0.57 (PSW, DW, MDMW); 2 (SMW)	.7 (HBSL)	Not detected in any well type

occurrence of the contaminants of potential concern is interpreted in a human-health context by considering factors such as detection frequency and well type. These three general steps are elucidated in the next three sections.

Step 1: Identify Human-Health Benchmarks and Compare to Measured Concentrations

The first step in interpreting water-quality data in a human-health context is to identify all applicable Federal (USEPA) and state human-health benchmarks, as well as HBSL values, for detected compounds, and to compare measured concentrations to these benchmarks. Historically, USGS has used USEPA MCL, Lifetime HA, and RSD values (defined in table 2) to assess water-quality conditions (Gilliom and others, 1998). For contaminants that have more than one of these three benchmarks available, the USGS has historically used the MCL, if available; otherwise, either the Lifetime HA (for noncarcinogens) or the RSD, usually at a 10^{-5} cancer risk level (for potential carcinogens), was used. For the few compounds with both a Lifetime HA and an RSD value, the lower value was used in order to be protective of both noncancer and cancer effects. USGS also historically has compared water-quality data to state standards and guidelines, where they exist, in state- and local-scale water-quality studies.

HBSL values supplement USEPA and state standards and guidelines for drinking water. The two-tiered HBSL approach for interpreting water-quality data in a human-health context was introduced in the section "Development and Use of Health-Based Screening Level Values" and is described in more detail in the "Tier 1: Benchmarks for Regulated Compounds" and the "Tier 2: Benchmarks for Unregulated Compounds" sections below. This two-tiered HBSL approach entails listing water-quality data for regulated compounds separately from unregulated compounds. In both Tier 1 and Tier 2 analyses, the listed water-quality data may include the contaminant name, number of samples collected, percentage of samples with detections, MRL values, human-health benchmarks, and measured concentrations.

Determining which measured concentrations (for example, maximum concentrations and median concentrations) to compare with human-health benchmarks depends, in part, on the hydrologic system being studied. Contaminant concentrations in ground-water systems tend to change relatively slowly as a function of time, and, depending on the objectives of the analysis and the nature of the data set, it may be appropriate to compare a variety of concentrations with human-health benchmarks (examples include median and maximum concentrations, a median-detected concentration (which excludes non-detected values), and (or) a range of percentiles). The median-detected concentration may be biased towards the high end of the concentration distribution, particularly when there are a substantial number of samples without detections, and comparisons between maximum detected concentrations and human-health benchmarks may be conservative (Toccalino and others, 2003). In data sets with low detection frequencies, comparisons of median concentrations and some percentile concentrations with human-health benchmarks have limited utility because these concentrations will be equivalent to non-detected values.

Tier 1 – Benchmarks for Regulated Compounds

For Tier 1 analysis, measured concentrations of regulated compounds are compared to drinking-water standards. In this study, there are two applicable drinking-water standards: USEPA MCL values and New Jersey State MCL values, both of which are legally enforceable (table 2). The State of New Jersey's drinking-water standards are equal to, or more stringent than, the USEPA standards. MCL values protect public health by limiting the levels of contaminants in drinking water. MCL values are established on the basis of health effects, but are not strictly health-based values. Analytical and best-available treatment technology limitations also are considered, and for noncarcinogens only, costs may be considered in the development of MCL values (New Jersey Department of Environmental Protection, 2000).

Tier 1 analysis begins with listing all detected, regulated compounds, along with their Federal and state MCL values. The USEPA and New Jersey MCL values (current as of 2004) used in this report for regulated pesticides and VOCs are provided in Appendix 1. The most current USEPA MCL values are published in the Code of Federal Regulations and in periodic USEPA compilations of drinking-water contaminants and their MCL values (U.S. Environmental Protection Agency, 2002b, 2003b, and 2004). Current New Jersey MCL values are available on the NJDEP web site (New Jersey Department of Environmental Protection, 2002). MCL values for other states typically are published on state drinking-water program web sites (for example see, Association of State Drinking Water Administrators, 2003).

Tier 2 – Benchmarks for Unregulated Compounds

For Tier 2 analysis, measured concentrations of unregulated compounds are compared to HBSL values. HBSL values are estimates of benchmark concentrations in water that may be of potential human-health concern. Measured concentrations are compared to HBSL values in lieu of USEPA OW Lifetime HA and RSD values; however, HBSL values typically are equivalent to USEPA OW Lifetime HA and RSD values, when available, because HBSL values were developed using USEPA OW methodologies and USEPA toxicity data. HBSL values may be different from published Lifetime HA or RSD values for compounds with USEPA toxicity values that are more recent than those used to develop Lifetime HA or RSD values. Additionally, HBSL values exist for some compounds with no published Lifetime HA or RSD values. HBSL values are described further in section "Development and Use of Health-Based Screening Level Values" and in table 2.

Table 2. Descriptions of human-health benchmarks related to drinking water used in this report.

[Maximum Contaminant Levels (Federal and State) are enforceable standards; the remainder of the listed benchmarks are unenforceable guidelines or public-health goals; USGS, U.S. Geological Survey; USEPA, U.S. Environmental Protection Agency; OW, Office of Water (USEPA); kg, kilogram; L, liter; ORD, Office of Research and Development (USEPA); µg/L, micrograms per liter; NJDEP, New Jersey Department of Environmental Protection]

Human-health benchmark	Acronym	Agency	Description	References
Health-Based Screening Level	HBSL	USGS	Estimates of benchmark concentrations (for noncarcinogens) or concentration ranges (for carcinogens) in water that (a) may be of potential human-health concern; (b) can be used as threshold values against which measured concentrations of contaminants in ambient water samples can be compared; and (c) are consistent with USEPA Office of Water methodologies for setting drinking-water Lifetime Health Advisory and Risk-Specific Dose values (U.S. Environmental Protection Agency, 1988 and 1993).	(Toccalino and others, 2003)
Maximum Contaminant Level (Federal)	USEPA MCL	USEPA (OW)	The maximum permissible level of a contaminant in water that is delivered to any user of a public water system. MCLs are set as close to Maximum Contaminant Level Goals (MCLGs) as feasible using the best available treatment technology and taking cost into consideration. The MCLG is the concentration of a contaminant in drinking water at which no known or anticipated adverse health effects occur and which allows an adequate margin of safety.	(U.S. Environmental Protection Agency, 2003a and 2004)
Lifetime Health Advisory	Lifetime HA	USEPA (OW)	The concentration of a contaminant in drinking water that is not expected to cause any adverse noncarcinogenic effects over a lifetime of exposure (70 years). The Lifetime HA is based on exposure of a 70-kg adult consuming 2 L of water per day, and assumes that only part (generally 20 percent) of the total exposure to a contaminant is from drinking water.	(U.S. Environmental Protection Agency, 1993 and 2004)
Risk-Specific Dose	RSD	USEPA (OW & ORD)	The concentration of a contaminant in drinking water that corresponds to a specific estimated lifetime cancer risk (typically 1 in 10,000, 1 in 100,000, or 1 in 1,000,000). The RSD is always associated with a specific cancer risk level. A related benchmark is the unit drinking-water risk, which is risk per microgram per liter concentration.	(U.S. Environmental Protection Agency, 2001 and 2004)
Maximum Contaminant Level (State)	New Jersey MCL	NJDEP	The maximum permissible level of a contaminant in water measured at the point of entry to the distribution system or at the free-flowing outlet of the ultimate user of a public water system or other water system to which State primary drinking water regulations apply. For carcinogens, the health-based goal is a 1 in 1,000,000 excess cancer risk over a lifetime of exposure; for noncarcinogens, the health-based goal is a level at which no known or anticipated health effects would be expected to occur.	(New Jersey Department of Environmental Protection, 2000)
Ground Water Quality Criteria	GWQC	NJDEP	Contaminant concentrations that, when not exceeded, will not prohibit or significantly impair the use of ground water for potable water or conversion to potable water through conventional water treatment. Values are human-health risk-based criteria based on the available evidence regarding each constituent's carcinogenicity or toxicity, as appropriate for the protection of potable-water use.	(New Jersey Department of Environmental Protection, 1993 and 2004a)
Interim Specific Ground Water Quality Criteria	Interim Specific GWQC	NJDEP	Contaminant concentrations in ground water for chemicals where a specific GWQC is not available. Values are based on the same methodologies and risk assessment approach applied to the development of the specific GWQC.	(New Jersey Department of Environmental Protection, 1993 and 2004b)

For Tier 2 analysis, measured concentrations of unregulated compounds also may be compared to state guideline values, if available. The State of New Jersey published two numerical criteria—the GWQC and the Interim Specific GWQC Criteria (table 2)—that were developed as part of the New Jersey Ground Water Quality Standards (GWQS). The GWQS specify the quality criteria (numerical values) and designated uses for ground water (New Jersey Department of Environmental Protection, 1993). Like HBSL values, GWQC and Interim Specific GWQC values also were developed using USEPA OW methodologies. NJDEP also publishes Interim Generic GWQC that are not health-based values, but are used as default values for synthetic organic chemicals (SOC) when no specific criterion exists or when published health information is lacking (New Jersey Department of Environmental Protection, 2004b). Interim Generic GWQC values are not included in table 2 or in the remainder of this report because they are not health-based values.

Tier 2 analysis begins with listing all detected, unregulated compounds, along with their applicable HBSL values and state-guideline values. The HBSL values used in this report (current as of August 2004) for unregulated pesticides and VOCs are provided in Appendix 2. HBSL values are updated on a monthly basis to incorporate any new or updated toxicity values published by USEPA. Up-to-date GWQC and Interim Specific GWQC values are available on NJDEP's web sites (New Jersey Department of Environmental Protection, 2004a and 2004b).

Step 2: Identify Contaminants of Potential Human-Health Concern Using Benchmark Quotients

The second step in interpreting water-quality data in a human-health context is to identify contaminants of potential human-health concern by assessing the differential between measured concentrations and human-health benchmarks. For ground-water data collected in this study, a **Benchmark Quotient** (BQ) value, the ratio of the measured concentration of a detected contaminant to its USEPA MCL value (for a regulated compound) or to its HBSL value (for an unregulated compound), was calculated for individual pesticides and VOCs. For regulated compounds with New Jersey MCL values but no USEPA MCL values, the BQ values were calculated using New Jersey MCL values. For unregulated carcinogens, the HBSL value used to calculate BQ values corresponds to a 10^{-6} cancer risk (that is, the low end of the HBSL concentration range). HBSL values were rounded to one significant figure to be consistent with USEPA OW practices (Toccalino and others, 2003); therefore, all BQ values also were rounded to one significant figure.

Different types of BQ values can be calculated for detected compounds; three types of BQ values were calculated for each well type in this study. Maximum BQ **(BQmax)** values were calculated for each detected compound (with a human-health benchmark) in each well type, where the BQmax value represents the maximum detected concentration of a compound in a given well type divided by the compound's MCL or HBSL value. Median BQ **(BQmed-det)** values were calculated for compounds with BQmax values greater than or equal to (≥) 0.1. BQmed-det values represent the median of detected concentrations of a compound (that is, the median value of all detected concentrations only) in a given well type divided by the MCL or HBSL value for the compound.

A third type of BQ value was calculated to represent the median of all samples (including non-detections) divided by the MCL or HBSL value **(BQmed-all)**, where non-detections were assigned a concentration equal to the MRL for a given compound. BQmed-all values are not presented in this report, because most detected compounds with human-health benchmarks were detected less than 50 percent of the time in any well type and therefore BQmed-all values are equivalent to the ratio of the MRL to the human-health benchmark.

In this report, **contaminants of potential human-health concern** are defined as pesticides and VOCs with maximum detected concentrations within a factor of 10 of applicable human-health benchmarks (that is, BQmax ≥ 0.1) in any of the three well types. The selection of 0.1 as the BQ threshold for identifying contaminants of potential human-health concern is consistent with various state and USEPA practices. For example, USEPA published a draft final rule defining a water-reference level as the level at or above which the agency wants to be informed of the presence of a pesticide in water resources. The water-reference level was further defined as 10 percent of the MCL or other applicable level in order to provide an early warning of potential problems with pesticides in water resources (U.S. Environmental Protection Agency, 1996). Furthermore, the USEPA final Federal Register notice on reporting requirements for risk/benefit information for pesticides indicated that, if a pesticide is detected in ground water, surface water, or finished drinking water, then the detections should be reported in three categories: (1) detections at levels greater than the MCL or other applicable criterion, (2) detections at levels greater than 10 percent of the MCL but not to exceed the MCL or other applicable criterion, and (3) detections at levels less than 10 percent of the MCL or other applicable criterion (U.S. Environmental Protection Agency, 2003c). In this report, the magnitude of pesticide and VOC detections in ground water, relative to their benchmark values, is reported in these same three categories.

Step 3: Interpret the Occurrence of Contaminants of Potential Human-Health Concern

The third step in interpreting water-quality data in a human-health context is to evaluate the occurrence of the contaminants of potential human-health concern (that is, those contaminants with BQmax ≥ 0.1) by considering five primary

factors. These five factors are (1) magnitude of the BQ values, (2) detection frequency, (3) MRL considerations, (4) well type and use of water, and (5) sources and physicochemical properties of the contaminants.

First, although contaminants of potential human-health concern are defined in this report as contaminants with BQmax ≥ 0.1, contaminants with BQ values ≥ 1 have more human-health importance than contaminants with BQ values < 1. BQ values ≥ 1 indicate that measured concentrations met or exceeded a human-health benchmark (MCL or HBSL value). For example, a BQ value of 10 indicates that the measured concentration of a chemical was 10-fold greater than the human-health benchmark; it does not mean that the chemical is 10-fold more toxic than a chemical with a BQ value equal to 1. BQ values less than 1 indicate that measured concentrations were less than the applicable human-health benchmarks. BQ values that are less than 1 also provide useful information about the potential for human-health effects. For example, a BQ value less than 0.001 indicates that measured concentrations of a contaminant were more than a factor of 1,000 less than the applicable human-health benchmark, and therefore, this contaminant is not likely to be of concern to human health. In contrast, a BQ value in the range of 0.1 to 1 indicates that the measured concentration of a contaminant was within a factor of 10 of the MCL or HBSL value. As a result, it may be desirable to monitor future concentrations of this contaminant to account for variability in sample collection and analysis, and to track trends in the occurrence of this contaminant over time.

Second, compounds that are frequently detected are more likely to be of concern than compounds that are detected infrequently. In this report, **frequently detected compounds** are defined as those compounds that are detected in at least 10 percent of samples from any given well type. This definition of frequently detected compounds is consistent with usage in a previously published report of the LINJ Study Unit (Stackelberg and others, 2000). This definition also generally follows USEPA human-health risk assessment guidance that discusses the evaluation of contaminants of potential concern based on frequency of detection (U.S. Environmental Protection Agency, 1989b). This USEPA guidance focuses assessments on contaminants that are consistently detected, rather than on those that are detected infrequently. The USEPA guidance provides an example in which assessments are focused on compounds detected in at least 5 percent of samples, assuming that at least 20 samples were collected (one detection in 20 samples equals a 5 percent frequency of detection), but this guidance also allows the use of a different detection frequency (U.S. Environmental Protection Agency, 1989b).

Third, contaminants of potential human-health concern and detection frequencies are evaluated in the context of MRL values for the analytical method used. If the MRL value for a contaminant is greater than the human-health benchmark for that contaminant, then (1) any detections of that contaminant will be greater than the human-health benchmark (that is, BQ value > 1), unless estimated concentrations less than the MRL are reported, and (2) there is the possibility that the contaminant could be present at concentrations that are of human-health concern (that is, BQ value ≥ 0.1), even in samples where that contaminant is not detected. In general, the detection frequency for a given contaminant will tend to decrease as the MRL increases. See the section "Interpreting Detection Frequencies" for additional considerations regarding the MRL in a human-health context.

Fourth, well type is important because it affects potential human exposure (through possible drinking-water consumption) to contaminants present in the water. The relevance of water-quality data from the public-supply, domestic, and monitoring wells considered in this study to human-health concerns differs markedly.

Ground-water samples collected from public-supply wells are relevant to human health because these water resources currently are used as drinking-water sources for large numbers of people. Ground water from public-supply wells typically is treated (disinfected) before it is consumed, however, the NAWQA Program primarily collects and analyzes raw water samples (that is, water sampled prior to treatment). If water from public-supply wells contains measured concentrations of contaminants that exceed MCL values, then the water supply is treated to remove the contaminants (New Jersey Department of Environmental Protection, 2000). Therefore, contaminants measured in raw water from public-supply wells may not be present at the same concentrations in the water consumed by the people who are served by those wells. Further, estimating the potential exposure to consumers of water from public-supply wells is complicated by the fact that public-supply distribution systems could contain water that is blended from multiple water sources. Beginning in 2004, the NAWQA Program's Source Water Quality Assessment component monitors both raw and treated ground-water samples.

Ground-water data collected from domestic wells are particularly relevant to human health because (1) the ground water is a current drinking-water resource and (2) these water resources typically are consumed with little or no treatment. Ground water from domestic wells is consumed by smaller numbers of people (typically one family per well) than ground water from public-supply wells (typically thousands of people per well). The estimation of the potential exposure to consumers of water from domestic wells is limited, however, because only one sample was collected per well; this prevents the estimation of representative exposure over time (this limitation also is true for the other well types).

In contrast, ground-water data collected from monitoring wells are not immediately relevant to human health because water from these wells is not consumed (non-potable wells). Although the water collected from monitoring wells is not a current source of drinking water, contamination in these wells can be both a contributor to, and a predictor of, future contaminant concentrations in deeper aquifers that may be used, now or in the future, for domestic and public supplies. Data from monitoring wells also can provide substantial insight about contaminant sources, their environmental fate and transport, and trends in concentrations over time.

Examining ground-water data by well type (as was done in this study) can provide regional water-quality information, as well as identify local concerns. For example, if a chemical is detected in only one well at a concentration greater than the MCL or HBSL value, this chemical may not have noteworthy regional importance, but it could have local importance.

Lastly, it also is useful to characterize the sources and physicochemical properties of contaminants that are identified as being of potential human-health concern, and (or) those that are frequently detected, to help understand potential human exposure to these contaminants. The physicochemical properties of a contaminant provide information about its fate and transport, biodegradability, persistence in water resources, and migration to other water resources. Such information helps in assessing the potential human exposure to a contaminant. Contaminants that are mobile and (or) persistent in the environment are of greater relevance to potential human exposure than contaminants that are not mobile and (or) that readily degrade in the environment. Contaminants that are highly water soluble, poorly sorbed to soil and aquifer matter, and highly persistent (resistant to degradation) pose the greatest likelihood of contaminating ground water. The sources and physicochemical properties of contaminants that were frequently detected in the LINJ Study Unit were described in detail by Stackelberg and others (2000), and therefore, are not explained in depth in this report.

All five of the factors described above need to be considered when interpreting water-quality data in a human-health context. Combinations of these factors help identify which detected contaminants could pose the greatest human-health concern. For example, contaminants that both (1) have measured concentrations that exceed human-health benchmarks and (2) are frequently detected in ground-water resources that are used for drinking water (that is, domestic or public-supply wells) are likely the most important contaminants from a human-health perspective. In contrast, contaminants that are detected infrequently and are present at concentrations well below their human-health benchmarks are least likely to be of concern. Other notable contaminants are those that are frequently detected in domestic or public-supply wells, but have no available toxicity data with which to calculate HBSL values. Identifying such compounds can assist Federal and state drinking-water agencies with prioritizing future data-collection and toxicity-evaluation activities.

Assessment of Ground-Water Quality in New Jersey

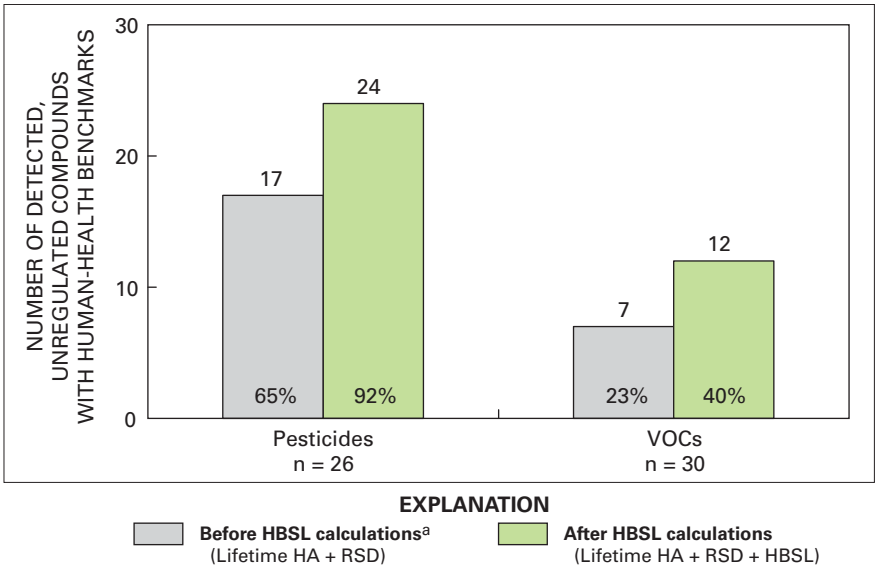
A total of 182 compounds (97 pesticides and 85 VOCs) were analyzed in this study, and 97 of these compounds were detected in samples from at least one of the three well types. The numbers of pesticides and VOCs that were analyzed and detected in the public-supply wells, domestic wells, and monitoring wells in the study area are summarized in table 3. The number of detected, unregulated pesticides and VOCs that have human-health benchmarks (before and after HBSL calculations) for comparison with measured concentrations also are provided in table 3 and illustrated in figure 3.

Table 3. Numbers of (1) pesticides and VOCs analyzed and detected in ground-water samples and (2) detected unregulated compounds with human-health benchmarks in ground-water samples from the Long Island-New Jersey Study Unit.

[VOC, volatile organic compound; HBSL, Health-Based Screening Level; PSW, public-supply well; DW, domestic well; MW, monitoring well; Lifetime HA, Lifetime Health Advisory; USEPA, U.S. Environmental Protection Agency; RSD, Risk-Specific Dose]

Well type	Number of compounds					
	All compounds		Detected compounds		Detected, unregulated compounds with human-health benchmarks	
	Analyzed	Detected	Regulated	Unregulated	Before HBSL calculations[1]	After HBSL calculations
				Pesticides		
PSW	47	15	4	11	8	10
DW	85	21	7	14	9	12
MW	97	30	8	22	17	21
				VOCs		
PSW	85	38	24	14	4	6
DW	85	47	27	20	4	9
MW	85	45	24	21	5	9

[1]Human-health benchmarks before HBSL calculations are Lifetime HA values from USEPA Office of Water and RSD values from either USEPA Office of Water or the USEPA Integrated Risk Information System database.



Detected, unregulated compounds with new HBSL values

Pesticides[b,c]

1. Acetochlor
2. Benfluralin
3. EPTC
4. Linuron
5. Napropamide
6. Norflurazon
7. Pendimethalin

VOCs

1. Acetone
2. Carbon disulfide
3. Ethyl ether
4. Isopropylbenzene
5. 1,1,2-trichloro-1,2,2-trifluoroethane

[a] Human-health benchmarks before HBSL calculations are Lifetime HA values from USEPA Office of Water and RSD values from either USEPA Office of Water or the USEPA Integrated Risk Information System database.

[b] Carbaryl has a USEPA Lifetime HA value (700 µg/L). Carbaryl also has a new HBSL range (40-4,000 µg/L) based on updated toxicity data published by USEPA Office of Pesticide Programs. Because carbaryl had a human-health benchmark before HBSL values were calculated, it is not included as a compound with a new benchmark in this figure.

[c] Diuron has a USEPA Lifetime HA (10 µg/L). Diuron also has a new HBSL range (2-200 µg/L) based on updated toxicity data published by USEPA Office of Pesticide Programs. Because diuron had a human-health benchmark before HBSL values were calculated, it is not included as a compound with a new benchmark in this figure.

[VOC, volatile organic compound; HBSL, Health-Based Screening Level; USEPA, U.S. Environmental Protection Agency; Lifetime HA, Lifetime Health Advisory; RSD, Risk-Specific Dose; %, percent; n, number of unregulated compounds detected; EPTC, 5-ethyl dipropylthiocarbamate]

Figure 3. Number of detected, unregulated pesticides and VOCs with human-health benchmarks before and after HBSL calculations in all well types in the Long Island-New Jersey Study Unit.

Step 1: Human-Health Benchmarks Identified and Compared to Measured Concentrations

Comparisons of measured ground-water contaminant concentration data with human-health benchmarks for pesticides and VOCs for all well types are presented in the following sections "Pesticides" and "Volatile Organic Compounds," respectively (tables 4-7). For each of these two contaminant classes, Tier 1 analysis for regulated compounds (that is, comparisons with USEPA and New Jersey drinking-water MCL values) is presented first (tables 4 and 6). Tier 2 analysis for unregulated compounds (that is, comparisons with HBSL values and with New Jersey GWQC and Interim Specific GWQC values) is presented second (tables 5 and 7).

Pesticides

Of the 97 total pesticides analyzed in this study, 38 (39 percent) were detected in at least one well type. Twelve of the 38 detected pesticides are regulated (that is, have a USEPA or New Jersey MCL value) and 26 are unregulated. Nearly all of the detected, unregulated pesticides (24 of 26) have human-health benchmarks, and seven of these benchmarks are new HBSL values (fig. 3).

Detection frequencies for pesticides ranged from less than 2 percent to 47 percent of samples in a given well type. Nine pesticides were frequently detected (that is, detected in 10 percent or more of samples) in samples from at least one of the well types (tables 4 and 5). All but one of these nine frequently detected pesticides has a human-health benchmark value; the exception is the herbicide metabolite, deethylatrazine.

Tier 1 – Regulated Pesticides

Twelve regulated pesticides were detected (out of 19 regulated pesticides analyzed) in ground-water samples collected from all well types (table 4). All regulated pesticides were detected at concentrations less than USEPA and New Jersey MCL values, with the exception of dinoseb in samples from monitoring wells (table 4). Dinoseb was detected in 4 of 72

monitoring-well samples, and measured concentrations exceeded the MCL in 2 of these 4 samples (table 4; fig. 4). Both of the detected concentrations (40 µg/L and 8 µg/L), which exceeded the USEPA and New Jersey MCL values of 7 µg/L, were estimated concentrations. The other two detections of dinoseb were at concentrations at least 100-fold below the MCL value. Estimated concentrations have greater uncertainty in their quantitation than concentrations that are not estimated, and this uncertainty also applies to the exceedance, particularly for the sample with 8 µg/L dinoseb, for which the estimated concentration was close to the MCL of 7 µg/L. Dinoseb was not detected in any samples from domestic wells and was not analyzed in public-supply well samples. Dinoseb was, however, analyzed and detected in public-supply well samples collected in a study by Vowinkel and others (1996).

Three regulated pesticides—atrazine, carbofuran, and simazine—were detected in all well types; however, none was detected at concentrations that exceeded USEPA or New Jersey MCL values (table 4). The maximum carbofuran concentration detected was more than 100-fold less than the MCL for all well types. Three regulated pesticides—atrazine, heptachlor epoxide, and simazine—were detected within a factor of 10 of their MCL values, but only in monitoring-well samples (table 4). Atrazine and simazine were frequently detected in all well types except for domestic wells; atrazine and simazine were detected in 9.9 percent and 8.6 percent, respectively, of the domestic wells. Heptachlor epoxide was analyzed only in monitoring-well samples, and was not frequently detected.

Tier 2 – Unregulated Pesticides

Twenty-six unregulated pesticides were detected (out of 78 unregulated pesticides analyzed) in ground-water samples collected from all well types, and measured concentrations were compared to HBSL values and New Jersey GWQC values, when available (table 5). Measured concentrations of two of these pesticides—dieldrin and diuron—met or exceeded their HBSL values in ground-water samples from at least one well type (table 5).

Dieldrin was detected in all well types, and all but 2 of the 31 measured concentrations of dieldrin exceeded the low end of the HBSL concentration range (10^{-6} cancer risk) and the New Jersey GWQC, which also is based on a 10^{-6} cancer risk (table 5; fig. 4). The low end of the HBSL concentration range and the New Jersey GWQC value for dieldrin are the same (both 0.002 µg/L) because New Jersey also uses USEPA OW methodologies for calculating GWQC values. Measured dieldrin concentrations in four monitoring-well samples also exceeded the high end of the HBSL concentration range (0.2 µg/L), which is based on a 10^{-4} cancer risk. In the two samples in which detected dieldrin concentrations did not exceed the low end of the HBSL concentration range, dieldrin was detected at concentrations within a factor of 10 of the HBSL (fig. 4).

The New Jersey practical quantitation level (PQL) for dieldrin is 0.03 µg/L (New Jersey Department of Environmental Protection, 2004a), which was exceeded in samples from three public-supply wells and six monitoring wells. The PQL is not a human-health benchmark but is equivalent to the concentration that can be reliably quantitated by NJDEP analytical methods (New Jersey Department of Environmental Protection, 2004b). The MRL for dieldrin analyzed in this study, using USGS methods, is 0.001 µg/L. This MRL is less than the low end of the HBSL concentration range and the New Jersey GWQC value (0.002 µg/L), thus allowing quantitation of dieldrin at concentrations that are relevant to human health.

Diuron was detected in 2 of 60 samples from domestic wells and in 5 of 72 samples from monitoring wells (table 5), but was not analyzed in public-supply well samples. The maximum detected concentration in domestic wells (1.9 µg/L) was approximately equal to the low end of the HBSL concentration range (2 µg/L). The maximum detected concentration of diuron in monitoring-well samples (2 µg/L) was an estimated concentration, equal to the low end of the HBSL concentration range (based on a 10^{-6} cancer risk) (table 5; fig. 4). In the five samples in which detected diuron concentrations were less than the low end of the HBSL concentration range, diuron was detected at concentrations within a factor of 10 of the HBSL (fig. 4). Because the maximum detected concentration in monitoring-well samples was an estimated concentration, which was equal to the human-health benchmark concentration, the uncertainty in this estimated concentration indicates that there also is uncertainty in the exceedance. Diuron has a Lifetime HA value of 10 µg/L; this value was not exceeded in any sample.

Five other unregulated pesticides with human-health benchmarks—carbaryl, *p,p*'-DDE, metolachlor, prometon, and terbacil—were detected in all well types; however, the detected concentrations were all well below their applicable HBSL values and New Jersey GWQC values (table 5). The maximum detected concentration of these five unregulated pesticides ranged from about 20-fold to more than1,000-fold less than their respective HBSL values.

Two unregulated pesticide analytes—deethylatrazine and fenuron—were detected but have no human-health benchmarks (Lifetime HA, RSD, HBSL, or GWQC values) to use for comparison against measured concentrations (table 5; Appendix 3). These compounds do not have human-health benchmarks because the toxicity data needed to calculate HBSL values are lacking. Deethylatrazine (a degradation product of the herbicides atrazine and propazine) was detected in all well types in 25 to 42 percent of the samples (table 5). Fenuron was analyzed in samples from domestic wells and monitoring wells, but was detected in only 1 of 60 domestic-well samples (table 5).

Table 4. Concentrations, detection frequencies, and MCL values for regulated pesticides detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.

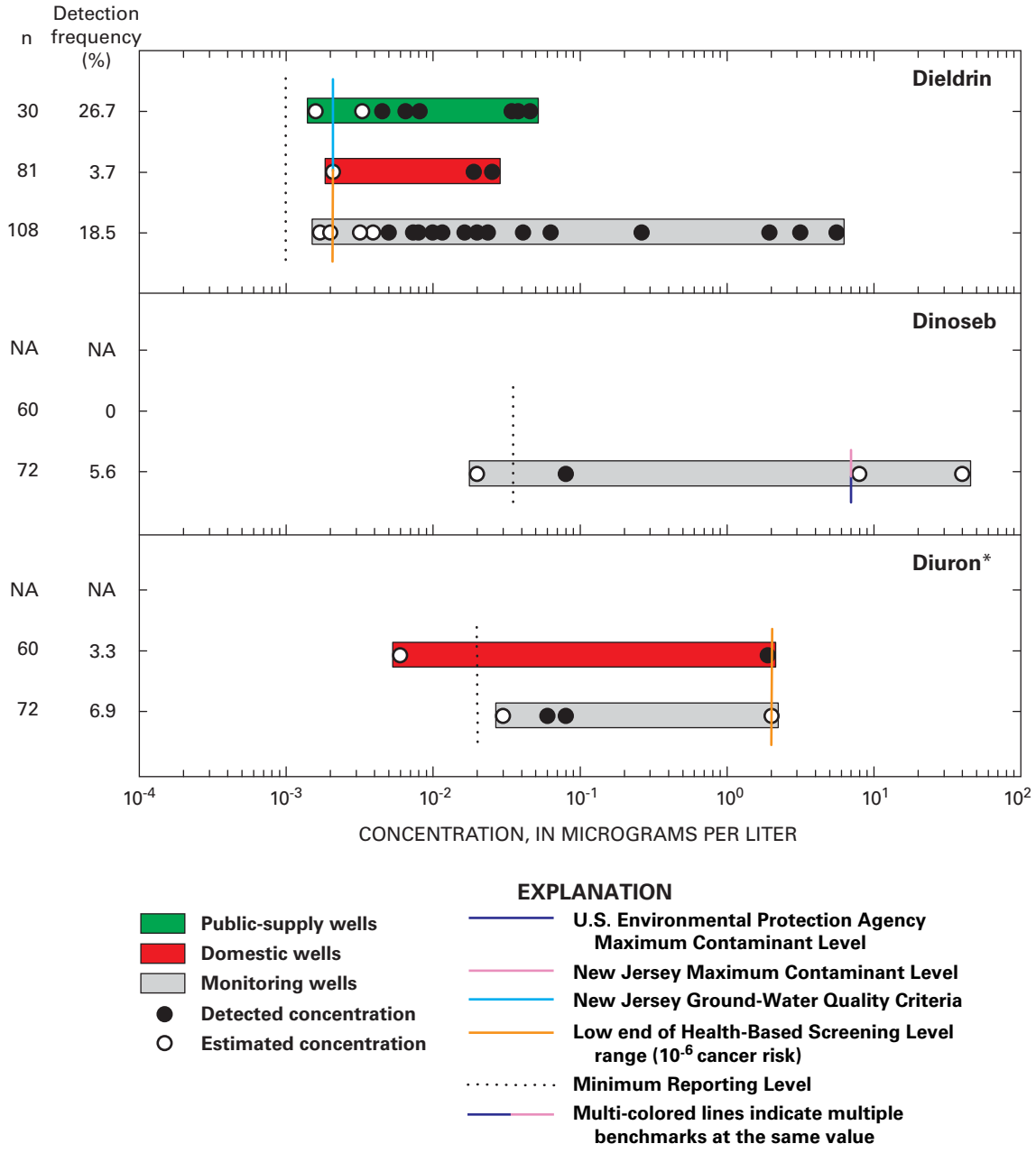
[MCL, Maximum Contaminant Level; **Bold type** indicates measured concentrations exceed USEPA or New Jersey MCL values; CASRN, Chemical Abstracts Service Registry Number; MRL, Minimum Reporting Level; µg/L, micrograms per liter; USEPA, U.S. Environmental Protection Agency; BQmax, Benchmark Quotient = ratio of maximum detected concentration to USEPA MCL value; <, less than; E, estimated value; 2,4-D, 2,4-dichlorophenoxyacetic acid; 2,4,5-TP, 2-(2,4,5-trichlorophenoxy) propionic acid]

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	USEPA MCL (µg/L)	New Jersey MCL (µg/L)	BQmax[1]
Public-supply wells (30 wells)									
Alachlor	15972-60-8	30	7	23.3	<0.002	0.0671	2	2	0.03
Atrazine	1912-24-9	30	9	30.0	<.001	.0341	3	3	.01
Carbofuran	1563-66-2	30	3	10.0	<.003	E.0773	40	40	.002
Simazine	122-34-9	30	8	26.7	<.005	.22	4	4	.06
Domestic wells (82 wells)									
Aldicarb sulfoxide	1646-87-3	60	1	1.7	<0.021	E0.23	4	4	0.06
Atrazine	1912-24-9	81	8	9.9	<.001	.0793	3	3	.03
Carbofuran	1563-66-2	81	2	2.5	<.003	E.218	40	40	.005
2,4-D	94-75-7	60	1	1.7	[2]<.15, <.035	.15	70	70	.002
Picloram	1918-02-1	60	1	1.7	<.05	E.05	500	500	.0001
Simazine	122-34-9	81	7	8.6	<.005	.265	4	4	.07
2,4,5-TP	93-72-1	60	1	1.7	<.021	.06	50	50	.001
Monitoring wells (108 wells)									
Alachlor	15972-60-8	108	3	2.8	<0.002	0.099	2	2	0.05
Atrazine	1912-24-9	108	51	47.2	<.001	.676	3	3	.2
Carbofuran	1563-66-2	108	6	5.6	<.003	E.173	40	40	.004
Chlordane, technical	12789-03-6	69	1	1.4	<.1	.1	[3]2	[3]0.5	.05
Dinoseb	88-85-7	72	4	5.6	<.035	**E40**	**7**	**7**	**6**
Heptachlor epoxide	1024-57-3	69	4	5.8	<.01	.07	0.2	0.2	.4
Lindane	58-89-9	108	1	0.9	<.004	.0128	0.2	0.2	.06
Simazine	122-34-9	108	41	38.0	<.005	1.38	4	4	.3

[1]BQmax values for regulated compounds were calculated using USEPA MCL values and were rounded to one significant figure.

[2]MRL value that applies to the largest number of samples (when more than one MRL exists for a given compound).

[3]USEPA MCL and New Jersey MCL are for chlordane (CASRN 57-74-9).



* Diuron has a USEPA Lifetime HA (10 µg/L). Diuron also has a new HBSL range (2-200 µg/L) based on updated toxicity data published by USEPA Office of Pesticide Programs.

[n, number of samples; %, percent; NA, not analyzed; USEPA, U.S. Environmental Protection Agency; HBSL, Health-Based Screening Level; Lifetime HA, Lifetime Health Advisory; µg/L, micrograms per liter]

Figure 4. Distributions of concentrations and detection frequencies of pesticides detected at concentrations that met or exceeded human-health benchmarks in at least one well type in the Long Island-New Jersey Study Unit.

Table 5. Concentrations, detection frequencies, and HBSL values for unregulated pesticides detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.

[HBSL, Health-Based Screening Level; **Bold type** indicates measured concentration exceeds New Jersey Ground-Water Quality Criteria (GWQC) or HBSL value; CASRN, Chemical Abstracts Service Registry Number; MRL, Minimum Reporting Level; µg/L, micrograms per liter; BQmax, Benchmark Quotient = ratio of maximum detected concentration to HBSL value or low end of HBSL range (10^{-6} risk); <, less than; --, not available; E, estimated value; USEPA, U.S. Environmental Protection Agency; RSD, Risk-Specific Dose; OPP, Office of Pesticide Programs (USEPA); q1*, cancer potency factor; Lifetime HA, Lifetime Health Advisory; *p*,*p*'-DDE, *p*,*p*'-dichlorodiphenyl dichloroethylene; IRIS, Integrated Risk Information System; SF, oral slope factor; PQL, practical quantitation level; RfD, oral reference dose; EPTC, 5-ethyl dipropylthiocarbamate]

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	New Jersey GWQC (µg/L)	HBSL concentration or range[1] (µg/L)	BQmax[2]	Basis for HBSL
Public-supply wells (30 wells)										
Acetochlor	34256-82-1	30	1	3.3	<0.002	0.0604	--	2 to 200	0.03	RSD approach using OPP q1*
Carbaryl	63-25-2	30	1	3.3	<.003	E.019	--	40 to 4,000	.0005	RSD approach using OPP q1* Note: Lifetime HA = 700 µg/L.
Cyanazine	21725-46-2	30	1	3.3	<.004	.0087	--	1	.009	Lifetime HA value
p,*p*'-DDE	72-55-9	30	2	6.7	<.006	E.00063	0.1	0.1 to 10	.006	RSD approach using IRIS SF
Deethylatrazine	6190-65-4	30	12	40.0	<.002	E.0234	--	--	--	No HBSL - no toxicity data available
Dieldrin	60-57-1	30	8	26.7	<.001	**.046**	**.002** PQL=0.03[3]	**0.002 to 0.2**	**20**	RSD approach using IRIS SF
Linuron	330-55-2	30	1	3.3	<.002	.0123	--	1	.01	Lifetime HA approach for Group C carcinogens using IRIS RfD
Metolachlor	51218-45-2	30	11	36.7	<.002	.671	--	100	.007	Lifetime HA value
Metribuzin	21087-64-9	30	2	6.7	<.004	.008	--	200	.00004	Lifetime HA value
Prometon	1610-18-0	30	3	10.0	<.018	E.0084	--	100	.00008	Lifetime HA value
Terbacil	5902-51-2	30	4	13.3	<.007	E.0978	--	90	.001	Lifetime HA value
Domestic wells (82 wells)										
Benfluralin	1861-40-1	81	1	1.2	<0.002	0.0057	--	2,000	0.000003	Lifetime HA approach using IRIS RfD
Carbaryl	63-25-2	81	2	2.5	<.003	E.539	--	40 to 4,000	.01	RSD approach using OPP q1* Note: Lifetime HA = 700 µg/L.
Dacthal	1861-32-1	81	1	1.2	<.002	E.0015	--	70	.00002	Lifetime HA value
p,*p*'-DDE	72-55-9	81	3	3.7	<.006	E.0056	.1	0.1 to 10	.06	RSD approach using IRIS SF
Deethylatrazine	6190-65-4	81	20	24.7	<.002	E.0801	--	--	--	No HBSL - no toxicity data available

Table 5. Concentrations, detection frequencies, and HBSL values for unregulated pesticides detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	New Jersey GWQC (µg/L)	HBSL concentration or range[1] (µg/L)	BQmax[2]	Basis for HBSL
Domestic wells (82 wells)—Continued										
Dieldrin	60-57-1	81	3	3.7	<0.001	**0.0251**	**0.002** PQL=0.03[3]	**0.002 to 0.2**	**10**	RSD approach using IRIS SF
Diuron	330-54-1	60	2	3.3	<.02	1.9	--	2 to 200	**1**	RSD approach using OPP q1* Note: Lifetime HA = 10 µg/L.
EPTC	759-94-4	81	1	1.2	<.002	.182	--	200	.0009	Lifetime HA approach using IRIS RfD
Fenuron	101-42-8	60	1	1.7	<.013	.05	--	--	--	No HBSL - no toxicity data available
Metolachlor	51218-45-2	81	3	3.7	<.002	.102	--	100	.001	Lifetime HA value
Napropamide	15299-99-7	81	1	1.2	<.003	.005	--	700	.000007	Lifetime HA approach using IRIS RfD
Prometon	1610-18-0	81	7	8.6	<.018	.025	--	100	.0002	Lifetime HA value
Terbacil	5902-51-2	81	3	3.7	<.007	E.891	--	90	.01	Lifetime HA value
Trifluralin	1582-09-8	81	1	1.2	<.002	.0066	--	5	.001	Lifetime HA value
Monitoring wells (108 wells)										
Bentazon	25057-89-0	72	2	2.8	<0.014	0.2	--	200	0.001	Lifetime HA value
Butylate	2008-41-5	108	1	.9	<.002	E.0025	--	400	.000006	Lifetime HA value
Carbaryl	63-25-2	108	7	6.5	<.003	E.781	--	40 to 4,000	.02	RSD approach using OPP q1* Note: Lifetime HA = 700 µg/L.
Cyanazine	21725-46-2	108	1	.9	<.004	.023	--	1	.02	Lifetime HA value
Dacthal	1861-32-1	108	1	.9	<.002	E.001	--	70	.00001	Lifetime HA value
p,*p*'-DDE	72-55-9	108	2	1.9	<.006	E.0018	.1	0.1 to 10	.02	RSD approach using IRIS SF
Deethylatrazine	6190-65-4	108	45	41.7	<.002	E.48	--	--	--	No HBSL - no toxicity data available
Dicamba	1918-00-9	72	1	1.4	<.035	E.45	--	200	.002	Lifetime HA value
Dieldrin	60-57-1	108	20	18.5	<.001	**5.6**	**.002** PQL=0.03[3]	**0.002 to 0.2**	**3,000**	RSD approach using IRIS SF

Table 5. Concentrations, detection frequencies, and HBSL values for unregulated pesticides detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	New Jersey GWQC (µg/L)	HBSL concentration or range[1] (µg/L)	BQmax[2]	Basis for HBSL
Monitoring wells (108 wells)—Continued										
Diuron	330-54-1	72	5	6.9	<0.02	**E2**	--	**2 to 200**	**1**	RSD approach using OPP q1* Note: Lifetime HA = 10 µg/L.
Fluometuron	2164-17-2	72	1	1.4	<.035	.04	--	90	.0004	Lifetime HA value
Linuron	330-55-2	108	1	.9	<.002	.024	--	1	.02	Lifetime HA approach for Group C carcinogens using IRIS RfD
Methomyl	16752-77-5	72	1	1.4	<.017	E.04	--	200	.0002	Lifetime HA value
Metolachlor	51218-45-2	108	30	27.8	<.002	.466	--	100	.005	Lifetime HA value
Metribuzin	21087-64-9	108	2	1.9	<.004	.159	--	200	.0008	Lifetime HA value
Napropamide	15299-99-7	108	1	.9	<.003	.043	--	700	.00006	Lifetime HA approach using IRIS RfD
Norflurazon	27314-13-2	72	1	1.4	<.024	.53	--	30	.02	Lifetime HA approach for Group C carcinogens using IRIS RfD
Pendimethalin	40487-42-1	108	3	2.8	<.004	.028	--	30	.0009	Lifetime HA approach for Group C carcinogens using IRIS RfD
Prometon	1610-18-0	108	20	18.5	<.018	4.83	--	100	.05	Lifetime HA value
Tebuthiuron	34014-18-1	108	6	5.6	<.01	E1.43	--	500	.003	Lifetime HA value
Terbacil	5902-51-2	108	5	4.6	<.007	E.495	--	90	.006	Lifetime HA value
Trifluralin	1582-09-8	108	2	1.9	<.002	.014	--	5	.003	Lifetime HA value

[1]HBSL range corresponds to a 10^{-6} to 10^{-4} cancer risk range for unregulated carcinogens.

[2]BQmax values for unregulated compounds were calculated using the HBSL concentration, or for carcinogens, the low end of the HBSL concentration range and were rounded to one significant figure.

[3]The Practical Quantitation Level (PQL) is the lowest concentration of a constituent that can be reliably achieved among laboratories within specified limits of precision and accuracy during routine laboratory operating conditions (New Jersey Department of Environmental Protection, 2001).

Volatile Organic Compounds

Of the 85 total VOCs analyzed in this study, 60 (71 percent) were detected in at least one well type. Half of the 60 detected VOCs are regulated, and half are unregulated. Twelve of the 30 detected, unregulated VOCs have human-health benchmarks, and 5 of these benchmarks are new HBSL values (fig. 3).

In general, VOCs were detected in ground-water samples more frequently than pesticides, with VOC detection frequencies ranging from less than 1 percent to 100 percent of samples from a given well type (tables 6 and 7). Twenty-two VOCs were frequently detected (that is, detected in 10 percent or more of samples) in samples from at least one of the well types (tables 6 and 7). All of the 22 frequently detected VOCs have human-health benchmarks (MCL or HBSL values).

Tier 1 – Regulated Volatile Organic Compounds

Thirty regulated VOCs were detected (out of 33 regulated VOCs analyzed) in ground-water samples collected from any one of the three well types (table 6). Four regulated VOCs had maximum detected concentrations that exceeded their USEPA or New Jersey MCL values in public-supply and (or) domestic well samples (table 6; fig. 5). These four VOCs are 1,2-dibromo-3-chloropropane, 1,2-dibromoethane, tetrachloroethylene (PCE), and trichloroethylene (TCE).

Measured concentrations of 1,2-dibromo-3-chloropropane in ground-water samples exceeded USEPA and New Jersey MCL values in the only sample in which it was detected (in 1 of 82 domestic-well samples) (table 6; fig. 5). The maximum detected concentration of 0.481 µg/L exceeded the USEPA and New Jersey MCL values of 0.2 µg/L by slightly more than two-fold. The MRL for 1,2-dibromo-3-chloropropane in domestic-well samples (0.214 µg/L) is slightly greater than the MCL value (table 6). Consequently, the possibility exists that some samples without detectable residues of 1,2-dibromo-3-chloropropane (as analyzed by this method) nonetheless could contain concentrations (greater than 0.2 but less than 0.214 µg/L) that exceed the MCL.

1,2-Dibromoethane was frequently detected (4 of 30 samples) in public-supply wells but was not detected in samples from any of the other well types (table 6). The maximum detected concentration of 1,2-dibromoethane (0.066 µg/L) in public-supply wells exceeded the USEPA and New Jersey MCL of 0.05 µg/L (table 6; fig. 5). The other three detections of 1,2-dibromoethane were at concentrations less than, but within a factor of 10 of, the MCL value; all four detected concentrations were estimated concentrations (table 6; fig. 5). Estimated concentrations have greater uncertainty in their quantitation, and this uncertainty also applies to the exceedance of a benchmark, particularly because the maximum detected concentration of 1,2-dibromoethane was close to the MCL (table 6; fig. 5).

PCE was frequently detected in all well types, but maximum detected concentrations exceeded the USEPA MCL (5 µg/L) and New Jersey MCL (1 µg/L) values in only 1 of 30 samples from public-supply wells (table 6; fig. 5). PCE was detected in 2 of 30 public-supply wells and 1 of 82 domestic wells at concentrations less than, but within a factor of 10 of, the USEPA MCL (fig. 5). PCE was detected in 9 of 30 public-supply wells, 5 of 82 domestic wells, and 5 of 108 monitoring wells at concentrations less than, but within a factor of 10 of, the New Jersey MCL (fig. 5).

TCE was frequently detected in all well types (table 6; fig. 5). Measured concentrations of TCE exceeded the USEPA MCL value (5 µg/L) in two samples (one sample each from the 30 public-supply and 82 domestic wells), and exceeded the New Jersey MCL value (1 µg/L) in four samples (two samples each from the 30 public-supply and 82 domestic wells) (table 6; fig. 5). TCE was detected in one of 30 public-supply wells and in one of 82 domestic wells at concentrations less than, but within a factor of 10 of, the USEPA MCL (fig. 5). TCE was detected in 10 of 30 public-supply wells, 3 of 82 domestic wells, and 2 of 108 monitoring wells at concentrations less than, but within a factor of 10 of, the New Jersey MCL (fig. 5).

In addition to PCE and TCE, 17 other regulated VOCs were detected in all well types. None were detected at concentrations that exceed USEPA or New Jersey MCL values, however, and nine of these regulated VOCs were detected at concentrations at least 10-fold less than the MCL values (table 6). Ten regulated VOCs—benzene, chloroethylene, 1,1-dichloroethane, 1,2-dichloroethane, 1,1-dichloroethene, *cis*-1,2-dichloroethylene, 1,2-dichloropropane, methyl *tert*-butyl ether (MTBE), methylene chloride, and trichloromethane—were detected within a factor of 10 of their human-health benchmarks for at least one well type. All of these VOCs were present in both public-supply wells and domestic wells (water that is consumed as drinking water), except methylene chloride, which was detected only in domestic wells (table 6).

Tier 2 – Unregulated Volatile Organic Compounds

Thirty unregulated VOCs were detected (out of 52 unregulated VOCs analyzed for) in ground-water samples collected from any well type, and measured concentrations were compared to HBSL values and to New Jersey GWQC and Interim Specific GWQC values, when available (tables 3 and 7). None of the unregulated VOCs were detected at concentrations that exceeded HBSL values (table 7). All unregulated VOCs were detected at concentrations at least 10-fold less than the HBSL values, and all but two VOCs (1-chloro-2-methylbenzene in public-supply wells and methyl chloride in monitoring wells) were detected at concentrations more than 100-fold less than the HBSL values. Isopropylbenzene and trichlorofluoromethane were the only unregulated VOCs with human-health benchmarks that were detected in all well types.

Table 6. Concentrations, detection frequencies, and MCL values for regulated VOCs detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.

[MCL, Maximum Contaminant Level; VOC, volatile organic compound; **Bold type** indicates measured concentrations exceed USEPA or New Jersey MCL values; CASRN, Chemical Abstracts Service Registry Number; MRL, Minimum Reporting Level; µg/L, micrograms per liter; USEPA, U.S. Environmental Protection Agency; BQmax, Benchmark Quotient = ratio of maximum detected concentration to USEPA (or New Jersey) MCL value; <, less than; --, not available; E, estimated value]

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	USEPA MCL (µg/L)	New Jersey MCL (µg/L)	BQmax[1]
Public-supply wells (30 wells)									
Benzene	71-43-2	30	5	16.7	[2]<0.032, <0.1	0.212	5	1	0.04
Bromodichloromethane	75-27-4	30	3	10.0	<.048	.369	[3]80	[3]80	.005
Bromoform	75-25-2	30	2	6.7	<.1, [2]<.104	.72	[3]80	[3]80	.009
Chlorobenzene	108-90-7	30	5	16.7	<.028	.128	100	50	.001
Chlorodibromomethane	124-48-1	30	2	6.7	<.18, [2]<.182	.595	[3]80	[3]80	.007
Chloroethylene	75-01-4	30	1	3.3	<.11, [2]<.112	E.054	2	2	.03
1,2-Dibromoethane	106-93-4	30	4	13.3	<.036	**E.066**	**0.05**	**0.05**	**1**
1,2-Dichlorobenzene	95-50-1	30	7	23.3	<.048	.729	600	600	.001
1,3-Dichlorobenzene	541-73-1	30	4	13.3	<.054	.104	--	600	.0002
1,4-Dichlorobenzene	106-46-7	30	10	33.3	<.05	.178	75	75	.002
1,1-Dichloroethane	75-34-3	30	13	43.3	<.066	.563	--	50	.01
1,2-Dichloroethane	107-06-2	30	2	6.7	<.13, [2]<.134	.299	5	2	.06
1,1-Dichloroethene	75-35-4	30	16	53.3	<.044	.722	7	2	.1
cis-1,2-Dichloroethylene	156-59-2	30	15	50.0	<.038	12.1	70	70	.2
trans-1,2-Dichloro-ethylene	156-60-5	30	4	13.3	<.032	.18	100	100	.002
1,2-Dichloropropane	78-87-5	30	3	10.0	<.068	1.42	5	5	.3
Methyl *tert*-butyl ether	1634-04-4	30	15	50.0	[2]<.112, <.17	1.41	--	70	.02
Tetrachloroethylene	127-18-4	30	22	73.3	[2]<.038, <.1	**71**	**5**	**1**	**10**
Tetrachloromethane	56-23-5	30	5	16.7	<.088	E.031	5	2	.006
1,1,1-Trichloroethane	71-55-6	30	21	70.0	<.032	1.13	200	30	.006
Trichloroethylene	79-01-6	30	17	56.7	<.038	**8.74**	**5**	**1**	**2**
Trichloromethane	67-66-3	30	30	100.0	<.052	2.5	[3]80	[3]80	.03
Xylenes (sum of isomers)[4]	1330-20-7	30	2	6.7	<.06, [2]<.064	.241	10,000	1,000	.00002

Table 6. Concentrations, detection frequencies, and MCL values for regulated VOCs detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	USEPA MCL (µg/L)	New Jersey MCL (µg/L)	BQmax[1]
Domestic wells (82 wells									
Benzene	71-43-2	82	3	3.7	<0.032, [2]<0.1	0.926	5	1	0.2
Bromodichloromethane	75-27-4	82	2	2.4	<.048	.331	[3]80	[3]80	.004
Bromoform	75-25-2	82	1	1.2	<.1, [2]<.104	E.044	[3]80	[3]80	.0006
Chlorobenzene	108-90-7	82	2	2.4	<.028	3.51	100	50	.04
Chloroethylene	75-01-4	82	1	1.2	<.11, [2]<.112	.386	2	2	.2
1,2-Dibromo-3-chloro-propane	96-12-8	82	1	1.2	<.21, [2]<.214	**.481**	**0.2**	**0.2**	**2**
1,2-Dichlorobenzene	95-50-1	82	2	2.4	<.048	.143	600	600	.0002
1,3-Dichlorobenzene	541-73-1	82	3	3.7	<.054	E.044	--	600	.00007
1,4-Dichlorobenzene	106-46-7	82	5	6.1	<.05	1.15	75	75	.02
1,1-Dichloroethane	75-34-3	82	10	12.2	<.066	.416	--	50	.008
1,2-Dichloroethane	107-06-2	82	1	1.2	<.13, [2]<.134	.205	5	2	.04
1,1-Dichloroethene	75-35-4	82	6	7.3	<.044	E.031	7	2	.004
cis-1,2-Dichloroethylene	156-59-2	82	2	2.4	<.038	2.99	70	70	.04
1,2-Dichloropropane	78-87-5	82	2	2.4	<.068	E.073	5	5	.01
Ethylbenzene	100-41-4	82	1	1.2	<.03	.103	700	700	.0001
Methyl *tert*-butyl ether	1634-04-4	82	25	30.5	<.112, [2]<.166, <.17	30.2	--	70	.4
Methylene chloride	75-09-2	82	2	2.4	<.38, [2]<.382	.674	5	3	.1
Naphthalene	91-20-3	82	1	1.2	<.25	2.47	--	300	.008
Styrene	100-42-5	82	1	1.2	<.042	E.005	100	100	.00005
Tetrachloroethylene	127-18-4	82	22	26.8	<.038, [2]<.102, <.1	.598	5	1	.1
Tetrachloromethane	56-23-5	82	2	2.4	<.088	.123	5	2	.02
Toluene	108-88-3	82	12	14.6	<.038, <.05, [2]<.054	E.069	1,000	1,000	.00007
1,1,1-Trichloroethane	71-55-6	82	19	23.2	<.032	.883	200	30	0.004
Trichloroethylene	79-01-6	82	12	14.6	<.038	**14.3**	**5**	**1**	**3**
Trichloromethane	67-66-3	82	56	68.3	<.052	13.5	[3]80	[3]80	.2
Xylenes (sum of isomers)[4]	1330-20-7	82	3	3.7	<.06, [2]<.064	.2356	10,000	1,000	.00002

Table 6. Concentrations, detection frequencies, and MCL values for regulated VOCs detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.—Continued

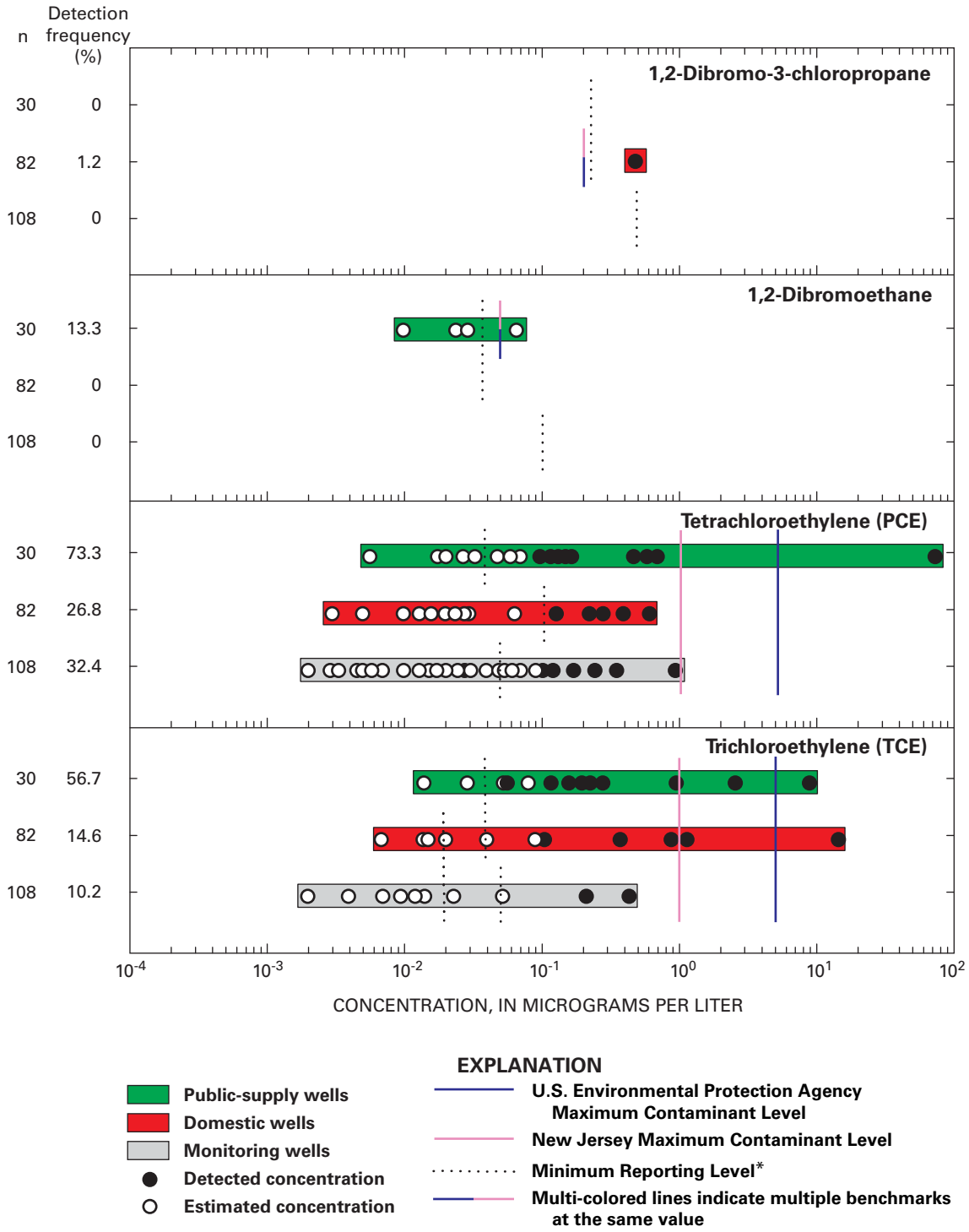
Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	USEPA MCL (µg/L)	New Jersey MCL (µg/L)	BQmax[1]
Monitoring wells (108 wells)									
Benzene	71-43-2	108	3	2.8	<0.032, [2]<0.05	0.333	5	1	0.07
Bromodichloromethane	75-27-4	108	5	4.6	<.048, [2]<.1	E.05	[3]80	[3]80	.0006
Bromoform	75-25-2	108	2	1.9	<.104, [2]<.2	E.04	[3]80	[3]80	.0005
Chlorobenzene	108-90-7	108	3	2.8	<.028, [2]<.05	E.012	100	50	.0001
Chlorodibromomethane	124-48-1	108	4	3.7	[2]<.1, <.182	E.04	[3]80	[3]80	.0005
1,2-Dichlorobenzene	95-50-1	108	7	6.5	<.048, [2]<.05	E.086	600	600	.0001
1,3-Dichlorobenzene	541-73-1	108	4	3.7	[2]<.05, <.054	E.043	--	600	.00007
1,4-Dichlorobenzene	106-46-7	108	7	6.5	<.05	.457	75	75	.006
1,1-Dichloroethane	75-34-3	108	9	8.3	[2]<.05, <.066	5.6	--	50	.1
1,2-Dichloroethane	107-06-2	108	2	1.9	[2]<.05, <.134	.69	5	2	.1
1,1-Dichloroethene	75-35-4	108	10	9.3	<.044, [2]<.1	.1	7	2	.01
cis-1,2-Dichloroethylene	156-59-2	108	3	2.8	<.038, [2]<.05	.305	70	70	.004
1,2-Dichloropropane	78-87-5	108	1	0.9	[2]<.05, <.068	E.04	5	5	.008
Ethylbenzene	100-41-4	108	3	2.8	<.03, [2]<.05	E.01	700	700	.00001
Methyl *tert*-butyl ether	1634-04-4	108	41	38.0	[2]<.1, <.112	43.8	--	70	.6
Naphthalene	91-20-3	108	1	0.9	[2]<.2, <.25	E.01	--	300	.00003
Styrene	100-42-5	108	1	0.9	<.042, [2]<.05	E.003	100	100	.00003
Tetrachloroethylene	127-18-4	108	35	32.4	<.038, [2]<.05	.946	5	1	.2
Toluene	108-88-3	108	8	7.4	<.038, [2]<.05	.133	1,000	1,000	.0001
1,1,1-Trichloroethane	71-55-6	108	34	31.5	<.032, [2]<.05	.64	200	30	.003
Trichloroethylene	79-01-6	108	11	10.2	<.038, [2]<.05	.434	5	1	.09
Trichloromethane	67-66-3	108	88	81.5	[2]<.05, <.052	5.6	[3]80	[3]80	.07
Xylenes (sum of isomers)[4]	1330-20-7	108	3	2.8	[2]<.05, <.064	E.03	10,000	1,000	.000003

[1]BQmax values for regulated compounds were calculated using USEPA MCL values. For compounds with New Jersey MCL values but no USEPA MCL values, the BQmax values were calculated using New Jersey MCL values. All BQmax values were rounded to one significant figure.

[2]MRL value that applies to the largest number of samples (when more than one MRL exists for a given compound).

[3]Under the USEPA 1998 final rule for disinfectants and disinfection byproducts, the total for trihalomethanes is 80 µg/L (U. S. Environmental Protection Agency, 2004).

[4]Sum of Xylenes = *m*- & *p*-xylene (CASRN 108-38-3 & 106-42-3) + *o*-xylene (CASRN 95-47-6).



* The MRL for some compounds varies for samples in a given well type. The most commonly reported MRL for each well type is shown in this figure.

[VOC, volatile organic compound; n, number of samples; %, percent; MRL, Minimum Reporting Level]

Figure 5. Distributions of concentrations and detection frequencies of VOCs detected at concentrations that met or exceeded human-health benchmarks in at least one well type in the Long Island-New Jersey Study Unit.

Table 7. Concentrations, detection frequencies, and HBSL values for unregulated VOCs detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.

[HBSL, Health-Based Screening Level; VOC, volatile organic compound; **Bold type** indicates measured concentration exceeds New Jersey Ground-Water Quality Criteria (GWQC); CASRN, Chemical Abstracts Service Registry Number; MRL, Minimum Reporting Level; µg/L, micrograms per liter; BQmax, Benchmark Quotient = ratio of maximum detected concentration to HBSL value; <, less than; --, not available; Lifetime HA, Lifetime Health Advisory; E, estimated value; IRIS, Integrated Risk Information System; RfD, oral reference dose; PQL, practical quantitation level; USEPA, U.S. Environmental Protection Agency]

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	New Jersey GWQC (µg/L)	HBSL concentration (µg/L)	BQmax[1]	Basis for HBSL
Public-supply wells (30 wells)										
1-Chloro-2-methyl-benzene	95-49-8	30	2	6.7	<0.042	2.73	--	100	0.03	Lifetime HA value
Dibromomethane	74-95-3	30	1	3.3	<.05	E.014	--	--	--	No HBSL - no toxicity data available
1,3-Dichloropropane	142-28-9	30	1	3.3	[2]<.116, <.12	E.056	--	--	--	No HBSL - no toxicity data available
Diisopropylether	108-20-3	30	1	3.3	<.098	.172	[3]20,000	--	--	No HBSL - no toxicity data available
Ethyl ether	60-29-7	30	1	3.3	<.17	.814	[3]1,000	1,000	.0008	Lifetime HA approach using IRIS RfD
1-Ethyl-2-methyl-benzene	611-14-3	30	1	3.3	<.1	.174	--	--	--	No HBSL - no toxicity data available
Isopropylbenzene	98-82-8	30	2	6.7	<.032	E.027	[3]800	700	.00004	Lifetime HA approach using IRIS RfD
1,1,1,2-Tetrachloro-ethane	630-20-6	30	1	3.3	<.044	E.011	10	70	.0002	Lifetime HA value
1,2,3,4-Tetramethyl-benzene	488-23-3	30	1	3.3	<.23	E.029	--	--	--	No HBSL - no toxicity data available
Trichlorofluoromethane	75-69-4	30	6	20.0	<.09, [2]<.092	.665	[3]2,000	2,000	.0003	Lifetime HA value
1,2,3-Trichloropropane	96-18-4	30	1	3.3	[2]<.07, <.16	**.164**	[3]**.005** [4]PQL=2	[5]40	.004	Lifetime HA value
1,2,3-Trimethylbenzene	526-73-8	30	1	3.3	<.12, [2]<.124	.186	--	--	--	No HBSL - no toxicity data available
1,2,4-Trimethylbenzene	95-63-6	30	1	3.3	<.056	E.055	--	--	--	No HBSL - no toxicity data available
1,3,5-Trimethylbenzene	108-67-8	30	1	3.3	<.044	E.017	--	--	--	No HBSL - no toxicity data available

Table 7. Concentrations, detection frequencies, and HBSL values for unregulated VOCs detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	New Jersey GWQC (µg/L)	HBSL concentration (µg/L)	BQmax[1]	Basis for HBSL
Domestic wells (82 wells)										
Acetone	67-64-1	82	1	1.2	[2]<4.9, <5	E6.88	700	6,000	0.001	Lifetime HA approach using IRIS RfD
n-Butylbenzene	104-51-8	82	1	1.2	[2]<.186, <.19	E.036	--	--	--	No HBSL - no toxicity data available
Carbon disulfide	75-15-0	82	8	9.8	<.08, [2]<.37	.216	[3]800	700	.0003	Lifetime HA approach using IRIS RfD
Chloroethane	75-00-3	82	1	1.2	<.12	.689	--	--	--	No HBSL - no toxicity data available
Dichlorodifluoro-methane	75-71-8	82	7	8.5	<.096, [2]<.138, <.14	E.95	[3]1,000	1,000	.001	Lifetime HA value
Diisopropylether	108-20-3	82	3	3.7	<.098	.159	[3]20,000	--	--	No HBSL - no toxicity data available
Ethyl ether	60-29-7	82	1	1.2	<.17	3.94	[3]1,000	1,000	.004	Lifetime HA approach using IRIS RfD
1-Ethyl-2-methyl-benzene	611-14-3	82	1	1.2	<.1	.255	--	--	--	No HBSL - no toxicity data available
Isopropylbenzene	98-82-8	82	1	1.2	<.032	.389	[3]800	700	.0006	Lifetime HA approach using IRIS RfD
Methyl chloride	74-87-3	82	3	3.7	<.25, [2]<.254	E.02	30	30	.0007	Lifetime HA value
Methyl ethyl ketone	78-93-3	82	1	1.2	<1.6, [2]<1.65	3.38	300	4,000	.0008	Lifetime HA value
Methyl iodide	74-88-4	82	1	1.2	<.076, [2]<.208, <.21	E.13	--	--	--	No HBSL - no toxicity data available
tert-pentyl methyl ether	994-05-8	82	1	1.2	<.11, [2]<.112	E.09	--	--	--	No HBSL - no toxicity data available
n-Propylbenzene	103-65-1	82	1	1.2	<.042	E.074	--	--	--	No HBSL - no toxicity data available
Tetrahydrofuran	109-99-9	82	2	2.4	<1.15, [2]<8.79, <9	7.97	[3]10 [4]PQL=20	--	--	No HBSL - no toxicity data available
1,2,3,4-Tetramethyl-benzene	488-23-3	82	1	1.2	<.23	.252	--	--	--	No HBSL - no toxicity data available

Table 7. Concentrations, detection frequencies, and HBSL values for unregulated VOCs detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	New Jersey GWQC (µg/L)	HBSL concentration (µg/L)	BQmax[1]	Basis for HBSL
Domestic wells (82 wells)—Continued										
1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	82	1	1.2	<0.032	E0.015	--	200,000	0.00000008	Lifetime HA approach using IRIS RfD
Trichlorofluoromethane	75-69-4	82	2	2.4	<.09, [2]<.092	1.06	[3]2,000	2,000	.0005	Lifetime HA value
1,2,4-Trimethylbenzene	95-63-6	82	1	1.2	<.056	E.056	--	--	--	No HBSL - no toxicity data available
1,3,5-Trimethylbenzene	108-67-8	82	1	1.2	<.044	E.051	--	--	--	No HBSL - no toxicity data available
Monitoring wells (108 wells)										
Acetone	67-64-1	108	3	2.8	<4.9, [2]<5	31.4	700	6,000	0.005	Lifetime HA approach using IRIS RfD
Bromobenzene	108-86-1	108	1	0.9	<.036, [2]<.05	E.0088	--	--	--	No HBSL - no toxicity data available
n-Butylbenzene	104-51-8	108	1	0.9	[2]<.05, <.186	E.019	--	--	--	No HBSL - no toxicity data available
sec-Butylbenzene	135-98-8	108	4	3.7	<.048, [2]<.05	.281	--	--	--	No HBSL - no toxicity data available
tert-Butylbenzene	98-06-6	108	3	2.8	[2]<.05, <.096	E.08	--	--	--	No HBSL - no toxicity data available
Carbon disulfide	75-15-0	108	41	38.0	[2]<.05, <.08	E.17	[3]800	700	.0002	Lifetime HA approach using IRIS RfD
1-Chloro-2-methylbenzene	95-49-8	108	1	0.9	<.042, [2]<.05	E.007	--	100	.00007	Lifetime HA value
Chloroethane	75-00-3	108	2	1.9	[2]<.1, <.12	.146	--	--	--	No HBSL - no toxicity data available
Dichlorodifluoromethane	75-71-8	108	5	4.6	<.096, [2]<.2	E4.3	[3]1,000	1,000	.004	Lifetime HA value
Diisopropylether	108-20-3	36	1	2.8	<.098	.485	[3]20,000	--	--	No HBSL - no toxicity data available
1-Ethyl-2-methylbenzene	611-14-3	108	1	0.9	[2]<.05, <.1	E.025	--	--	--	No HBSL - no toxicity data available

Table 7. Concentrations, detection frequencies, and HBSL values for unregulated VOCs detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	Number of samples	Number of samples with detections	Percentage of samples with detections	MRL (µg/L)	Maximum detected concentration (µg/L)	New Jersey GWQC (µg/L)	HBSL concentration (µg/L)	BQmax[1]	Basis for HBSL
Monitoring wells (108 wells)—Continued										
Isopropylbenzene	98-82-8	108	1	0.9	<0.032, [2]<0.05	E0.042	[3]800	700	0.00006	Lifetime HA approach using IRIS RfD
Methyl chloride	74-87-3	108	15	13.9	[2]<.2, <.254	E1.9	30	30	.06	Lifetime HA value
Methyl ethyl ketone	78-93-3	108	4	3.7	<1.65, [2]<5	7.06	300	4,000	.002	Lifetime HA value
Methyl iodide	74-88-4	108	6	5.6	[2]<.05, <.076	E.17	--	--	--	No HBSL - no toxicity data available
1-Methyl-4-isopropyl-benzene	99-87-6	108	5	4.6	[2]<.05, <.11	.71	--	--	--	No HBSL - no toxicity data available
tert-Pentyl methyl ether	994-05-8	108	3	2.8	[2]<.1, <.112	E.02	--	--	--	No HBSL - no toxicity data available
Tetrahydrofuran	109-99-9	108	2	1.9	<1.15, [2]<5	E2.66	[3]10 [4]PQL=20	--	--	No HBSL - no toxicity data available
1,1,2-Trichloro-1,2,2-Trifluoroethane	76-13-1	108	1	0.9	<.032, [2]<.05	.12	--	200,000	.0000006	Lifetime HA approach using IRIS RfD
Trichlorofluoromethane	75-69-4	108	11	10.2	<.092, [2]<.1	17	[3]2,000	2,000	.008	Lifetime HA value
1,2,4-Trimethylbenzene	95-63-6	108	1	0.9	[2]<.05, <.056	E.003	--	--	--	No HBSL - no toxicity data available

[1]BQmax values for unregulated compounds were calculated using the HBSL concentration and were rounded to one significant figure.

[2]MRL value that applies to the largest number of samples (when more than one MRL exists for a given compound).

[3]New Jersey Interim Specific GWQC based on the methodologies and risk assessment approach contained in the ground-water quality standards.

[4]The Practical Quantitation Level (PQL) is the lowest concentration of a constituent that can be reliably achieved among laboratories within specified limits of precision and accuracy during routine laboratory operating conditions (New Jersey Department of Environmental Protection, 2001).

[5]HBSL based on Lifetime HA value; 1,2,3-trichloropropane has been found to cause cancer in laboratory animals and an IRIS profile is currently being developed by USEPA (J.M. Donohue, U.S. Environmental Protection Agency, written commun., 2003).

One unregulated VOC, 1,2,3-trichloropropane, was detected in 1 of 30 samples from public-supply wells at a concentration that exceeded the New Jersey Interim Specific GWQC value (0.005 µg/L) (table 7). New Jersey's Interim Specific GWQC values are health-based criteria established by NJDEP for chemicals without specific GWQC (table 2). The maximum detected concentration of 1,2,3-trichloropropane, however, was approximately 200-fold less than the HBSL for this compound (40 µg/L), which was set equal to the USEPA Lifetime HA value. The HBSL and Interim Specific GWQC values for 1,2,3-trichloropropane differ because they are based on two different toxicity values. The HBSL is based on the oral **reference dose** value published in the USEPA IRIS database. Carcinogenicity data for 1,2,3-trichloropropane are not currently available in the IRIS database; however, an IRIS profile is being developed by USEPA because 1,2,3-trichloropropane has been found to cause cancer in laboratory animals (J.M. Donohue, U.S. Environmental Protection Agency, written commun., 2003). In contrast, the New Jersey Interim Specific GWQC value was calculated using an oral cancer **slope factor** value from USEPA HEAST (G.B. Post, New Jersey Department of Environmental Protection, written commun., 2003). 1,2,3-Trichloropropane is listed in HEAST as a B2 carcinogen on the basis of the results of a 1993 National Toxicology Program study (National Toxicology Program, 1993), which concluded that there was clear evidence of carcinogenicity in rats and mice.

Eighteen detected unregulated VOCs have no human-health benchmarks (Lifetime HA, RSD, HBSL, GWQC, or Interim Specific GWQC values) to use for comparison against measured concentrations (table 7; Appendix 3). These 18 VOCs do not have human-health benchmarks because the toxicity data needed to calculate HBSL values are lacking. None of these 18 VOCs were frequently detected, but 3 (diisopropylether, 1-ethyl-2-methylbenzene, and 1,2,4-trimethylbenzene) were detected in all well types (table 7).

Step 2: Contaminants of Potential Human-Health Concern Identified

Pesticides and VOCs were identified as being of potential human-health concern if maximum detected concentrations were within a factor of 10 of their human-health benchmarks (that is, BQmax ≥ 0.1) for any well type (see section "Identify Contaminants of Potential Human-Health Concern Using Benchmark Quotients"). BQmax values were calculated for all detected pesticides and VOCs with human-health benchmarks (tables 4-7). Twenty contaminants (6 pesticides and 14 VOCs) were identified as being of potential human-health concern because they had BQmax values ≥ 0.1 (BQmax range, 0.1-3,000) for at least one well type (table 8; figs. 6 and 7).

Most detected contaminants with human-health benchmarks (30 of 36 pesticides and 27 of 41 VOCs) were detected at concentrations more than10-fold less than human-health benchmarks (that is, BQmax < 0.1). More than half (41 of 77, or 53 percent) of detected pesticides and VOCs with human-health benchmarks had BQ values < 0.01 (that is, more than 100-fold less than human-health benchmarks) (tables 4-7).

Step 3: Occurrence of Contaminants of Potential Human-Health Concern Interpreted

Interpretation of the occurrence of contaminants of potential human-health concern (that is, those contaminants with BQ values ≥ 0.1) entails the consideration of five primary factors: (1) magnitude of the BQ values, (2) detection frequency, (3) MRL considerations, (4) well type and use of water, and (5) sources and physicochemical properties of the contaminants.

Magnitude of BQ Values and Detection Frequency

BQmax and BQmed-det values and detection frequencies for each of the 20 contaminants with BQmax ≥ 0.1 are listed in table 8 for all three well types. Because comparisons between maximum detected concentrations and human-health benchmarks (BQmax) may be conservative, the distributions of all detections of these 20 contaminants were examined. The distributions of BQ values and the detection frequencies for the 6 pesticides and 14 VOCs of potential human-health concern are shown in figures 6 and 7, respectively, and are discussed further in section "Patterns of Occurrence." Thirteen of the 20 contaminants of potential human-health concern were frequently detected in at least one well type (table 8).

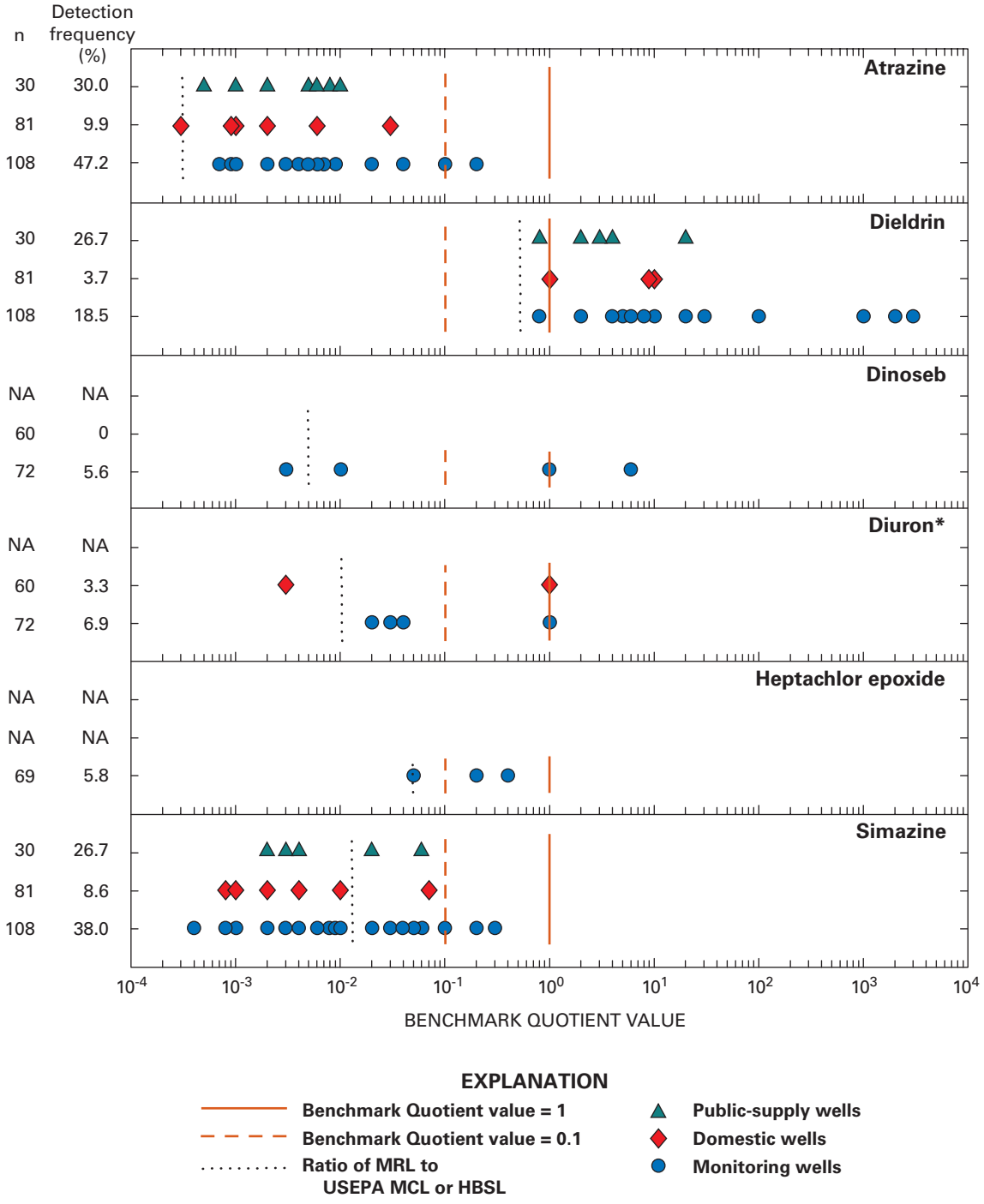
Seven of the 20 contaminants of potential human-health concern (dieldrin, dinoseb, diuron, 1,2-dibromo-3-chloropropane, 1,2-dibromoethane, PCE, and TCE) had maximum detected concentrations that met or exceeded human-health benchmarks (that is, BQmax ≥ 1) for at least one well type (table 8). The remaining 13 contaminants of potential human-health concern had measured concentrations that were less than, but within a factor of 10 of, the applicable human-health benchmarks (that is, 1 > BQmax ≥ 0.1) for all well types (table 8).

Only 2 of the 20 contaminants of potential human-health concern (dieldrin and 1,2-dibromo-3-chloropropane) had BQmed-det values ≥ 1 for at least one well type, indicating that the median of detected concentrations met or exceeded human-health benchmarks. For dieldrin, this was a result of measured concentrations exceeding the low end of the HBSL concentration range in most of the samples in which it was detected (figs. 4 and 6). In contrast, 1,2-dibromo-3-chloropropane was detected in only one sample from domestic wells, so its BQmed-det value is the same as its BQmax value (figs. 5 and 7). The median of detected concentrations were within a factor of 10 of human-health benchmarks (1 > BQmed-det ≥ 0.1) for six additional contaminants of potential human-health concern (dinoseb, heptachlor epoxide, diuron, chloroethylene, 1,2-dibromoethane, and methylene chloride) for at least one well type; most of these six contaminants had low detection frequencies, hence the BQmed-det values were similar (or equivalent) to the BQmax values.

Table 8. Detection frequencies and BQmax and BQmed-det values for pesticides and VOCs detected at concentrations within a factor of 10 of human-health benchmarks in samples from public-supply wells, domestic wells, and (or) monitoring wells in the Long Island-New Jersey Study Unit.

[Each compound has a BQmax greater than or equal to 0.1 in at least one well type; BQmax, Benchmark Quotient = ratio of maximum detected concentration to human-health benchmark value; BQmed-det, Benchmark Quotient = ratio of median of detected concentrations to human-health benchmark value; VOC, volatile organic compound; **Bold red type** indicates Benchmark Quotient (BQ) ≥1; ***Bold blue italic type*** indicates 0.1 ≤ BQ < 1; ≥, greater than or equal to; ≤, less than or equal to; <, less than; CASRN, Chemical Abstracts Service Registry Number; n, number of samples; %, percent; NA, not analyzed; ND, not detected]

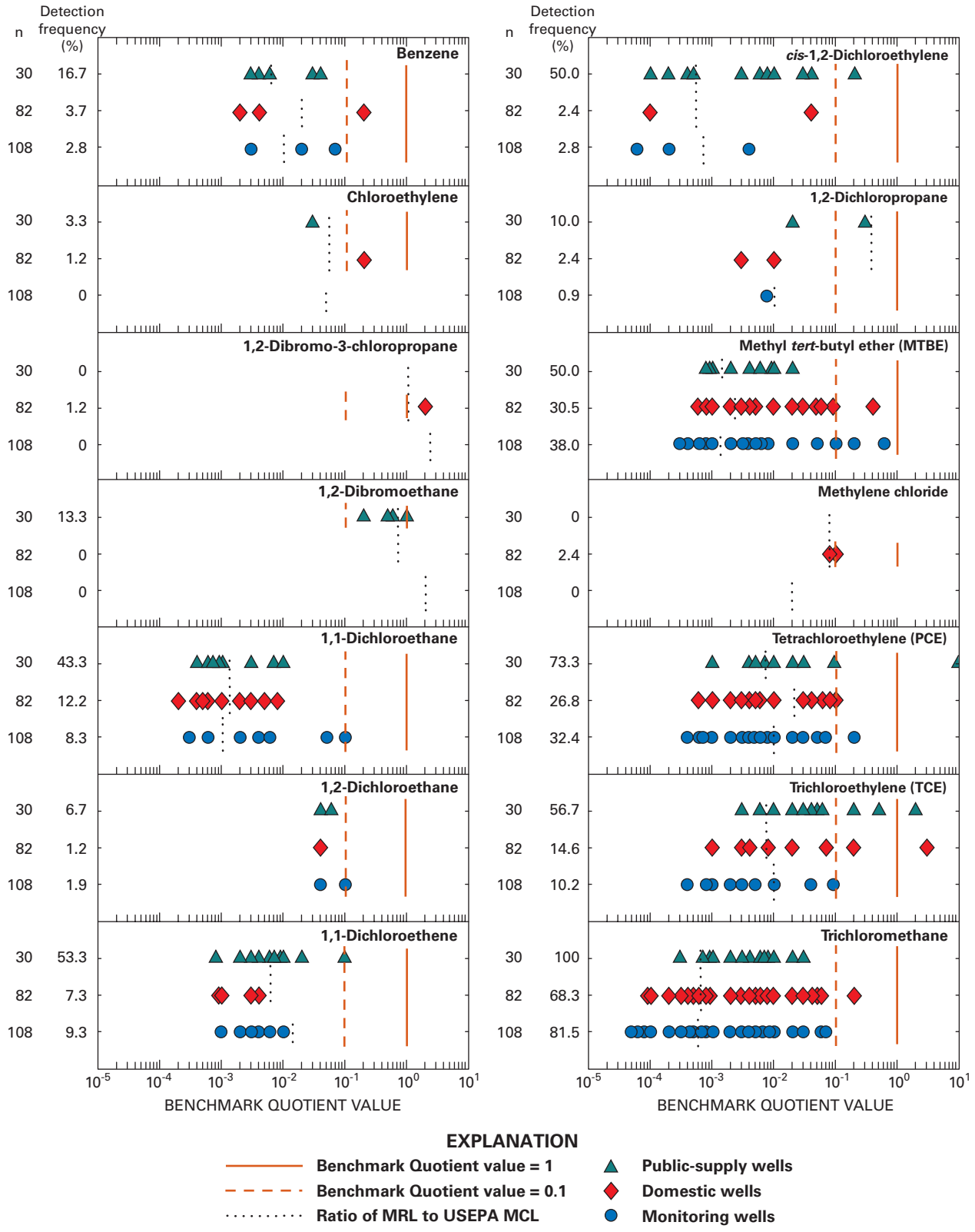
Compound	CASRN	Regulated or unregulated	Public-supply wells				Domestic wells				Monitoring wells			
			n	Detection frequency (%)	BQmax	BQmed-det	n	Detection frequency (%)	BQmax	BQmed-det	n	Detection frequency (%)	BQmax	BQmed-det
Pesticides														
Atrazine	1912-24-9	Regulated	30	30.0	0.01	0.006	81	9.9	0.03	0.002	108	47.2	***0.2***	0.002
Dinoseb	88-85-7	Regulated	NA	NA	NA	NA	60	ND	ND	ND	72	5.6	**6**	***.6***
Heptachlor epoxide	1024-57-3	Regulated	NA	NA	NA	NA	NA	NA	NA	NA	69	5.8	***.4***	***.1***
Simazine	122-34-9	Regulated	30	26.7	.06	.003	81	8.6	.07	.004	108	38.0	***.3***	.009
Dieldrin	60-57-1	Unregulated	30	26.7	**20**	**4**	81	3.7	**10**	**9**	108	18.5	**3,000**	**9**
Diuron	330-54-1	Unregulated	NA	NA	NA	NA	60	3.3	**1**	***.5***	72	6.9	**1**	.03
VOCs														
Benzene	71-43-2	Regulated	30	16.7	0.04	0.006	82	3.7	***0.2***	0.004	108	2.8	0.07	0.02
Chloroethylene	75-01-4	Regulated	30	3.3	.03	.03	82	1.2	***.2***	***.2***	108	ND	ND	ND
1,2-Dibromo-3-chloro-propane	96-12-8	Regulated	30	ND	ND	ND	82	1.2	**2**	**2**	108	ND	ND	ND
1,2-Dibromoethane	106-93-4	Regulated	30	13.3	**1**	***.5***	82	ND	ND	ND	108	ND	ND	ND
1,1-Dichloroethane	75-34-3	Regulated	30	43.3	.01	.0007	82	1.2	.04	.04	108	8.3	***.1***	.002
1,2-Dichloroethane	107-06-2	Regulated	30	6.7	.06	.05	82	1.2	.04	.04	108	1.9	***.1***	.09
1,1-Dichloroethene	75-35-4	Regulated	30	53.3	***.1***	.005	82	7.3	.004	.003	108	9.3	.01	.003
cis-1,2-Dichloro-ethylene	156-59-2	Regulated	30	50.0	***.2***	.003	82	2.4	.04	.02	108	2.8	.004	.0002
1,2-Dichloropropane	78-87-5	Regulated	30	10.0	***.3***	.02	82	2.4	.01	.009	108	.9	.008	.008
Methyl *tert*-butyl ether (MTBE)	1634-04-4	Regulated	30	50.0	.02	.004	82	30.5	***.4***	.004	108	38.0	***.6***	.003
Methylene chloride	75-09-2	Regulated	30	ND	ND	ND	82	2.4	***.1***	***.1***	108	ND	ND	ND
Tetrachloroethylene (PCE)	127-18-4	Regulated	30	73.3	**10**	.02	82	26.8	***.1***	.005	108	32.4	***.2***	.004
Trichloroethylene (TCE)	79-01-6	Regulated	30	56.7	**2**	.04	82	14.6	**3**	.01	108	10.2	.09	.002
Trichloromethane	67-66-3	Regulated	30	100	.03	.002	82	68.3	***.2***	.002	108	81.5	.07	.0008



* Diuron has a USEPA Lifetime HA (10 µg/L). Diuron also has a new HBSL range (2-200 µg/L) based on updated toxicity data published by USEPA Office of Pesticide Programs. The BQ values for diuron in this figure were calculated using an HBSL of 2 µg/L.

[BQ, Benchmark Quotient = ratio of detected concentration to human-health benchmark value; n, number of wells; %, percent; NA, not analyzed; MRL, Minimum Reporting Level; USEPA, U.S. Environmental Protection Agency; MCL, Maximum Contaminant Level; HBSL, Health-Based Screening Level; Lifetime HA, Lifetime Health Advisory; µg/L, micrograms per liter]

Figure 6. Distributions of Benchmark Quotient values and detection frequencies, by well type, for pesticides detected at concentrations within a factor of 10 of their human-health benchmarks in the Long Island-New Jersey Study Unit.



[BQ, Benchmark Quotient = ratio of detected concentration to human-health benchmark value; VOC, volatile organic compound; n, number of wells; %, percent; MRL, Minimum Reporting Level; USEPA, U.S. Environmental Protection Agency; MCL, Maximum Contaminant Level]

Figure 7. Distributions of Benchmark Quotient values and detection frequencies, by well type, for VOCs detected at concentrations within a factor of 10 of their human-health benchmarks in the Long Island-New Jersey Study Unit.

MRL Considerations

For 18 of the 20 contaminants of potential human-health concern, analytical MRL values were less than their HBSL or MCL values (tables 1 and 4-6), enabling the quantitation of these contaminants at concentrations that are relevant to human health. The exceptions are 1,2-dibromoethane and 1,2-dibromo-3-chloropropane, which had MRL values greater than or near their MCL values, resulting in benchmark exceedance rates and BQ values that have higher uncertainty than those for the other measured contaminants.

Well Type and Use of Water

Well type affects potential human exposure (through possible drinking-water consumption) to contaminants present in the ground water. Each of the well types considered in this study (see section "Well Networks") provides water-quality data of varying relevance to potential human-health concerns; water-quality data from each well type are discussed separately below. In this study, ground-water quality data were collected from multiple aquifers and land-use areas, in addition to multiple well types. Domestic-well samples were collected from three sampling regions (aquifers) and monitoring-well samples were collected from four land-use areas. In this study, therefore, the occurrence of contaminants is discussed as a function of well type, aquifer, and land use. The occurrence of three pesticides (dieldrin, dinoseb, and diuron) and four VOCs (1,2-dibromo-3-chloropropane, 1,2-dibromoethane, PCE, and TCE) with maximum detected concentrations that met or exceeded human-health benchmarks is summarized by well type, aquifer, and land use in table 9 and is discussed further in the following three sections.

Occurrence by Well Type

The patterns of pesticide and VOC detection frequencies in relation to BQmax values varied considerably among well types (figs. 8a and 8b). Pesticides and VOCs tended to have higher detection frequencies in public-supply wells than in the other well types. In public-supply wells, one pesticide (dieldrin) and three VOCs (1,2-dibromoethane, PCE, and TCE) were frequently detected and detected at concentrations that exceeded their human-health benchmark values (BQmax $\geq$ 1) (figs. 8a and 8b). Three additional VOCs (1,1-dichloroethene, *cis*-1,2-dichloroethylene, and 1,2,-dichloropropane) were frequently detected in public-supply wells and had BQmax values greater than 0.1 and less than 1 (fig. 8b).

In domestic wells, two pesticides (diuron and dieldrin) were detected at concentrations that met or exceeded their human-health benchmarks, but both were detected infrequently (fig. 8a). Only TCE was both frequently detected in domestic-well samples and exceeded its benchmark (BQmax = 3) in domestic wells. Measured concentrations of 1,2-dibromo-3-chloropropane exceeded its benchmark in domestic wells (BQmax = 2), but was not frequently detected (fig. 8b).

Detection frequencies of both pesticides and VOCs were higher in public-supply wells than in domestic wells, most likely because public-supply wells withdraw larger volumes of water from the aquifer. Consequently, public-supply wells capture recharge from relatively large contributing areas at the land surface (Stackelberg and others, 2000). In contrast, small volumes of water recharged from relatively small areas at the land surface are withdrawn at low rates from domestic wells.

More pesticides and VOCs combined were detected at concentrations within a factor of 10 of human-health benchmarks (BQmax $\geq$ 0.1) in domestic wells (10 compounds) than in public-supply wells (7 compounds) (figs. 8a and 8b). More pesticides were analyzed in samples from domestic wells (85) than public-supply wells (47); however, considering only compounds analyzed in samples from both well types, domestic wells contained more compounds with a BQmax greater than or equal to 0.1 (9 compounds) than public-supply wells (7 compounds). This finding is important because water from domestic wells typically is consumed directly without treatment.

Because ground water from both public-supply wells and domestic wells currently is used as drinking water, comparisons among the BQmax values for pesticides and VOCs were made between these two well types in the same aquifer, the Kirkwood-Cohansey aquifer system (figs. 9a and 9b). Eight pesticides and 19 VOCs with human-health benchmarks were detected in samples from the 30 public-supply wells and the 30 domestic wells in the Kirkwood-Cohansey aquifer system. Analysis of the paired BQmax values for these 8 pesticides and 19 VOCs using the Mann-Whitney test indicated that BQmax values for one well type were not significantly different from the BQmax values for the other well type. The results of these statistical tests were the same when pesticides and VOCs that were detected in only one of the two well types were included.

In monitoring wells, only one pesticide (dieldrin) was frequently detected and detected at concentrations that exceeded its benchmark value (BQmax = 3,000). Two additional pesticides (diuron and dinoseb) were not frequently detected but were detected at concentrations that met or exceeded their human-health benchmarks (BQmax = 1 and 6, respectively) (fig. 8a). No VOCs were detected in monitoring-well samples at concentrations that exceeded their benchmark values. Seven contaminants (three pesticides and four VOCs) were detected in monitoring-well samples at concentrations less than, but within a factor of 10 of, human-health benchmarks (1 > BQmax $\geq$ 0.1) (figs. 8a and 8b).

One pesticide (deethylatrazine) was frequently detected in all well types, but it has no human-health benchmark with which to compare measured concentrations. No VOCs without human-health benchmarks were frequently detected in any well type.

Table 9. Frequency of detection and frequency of exceedance of human-health benchmarks for pesticides and VOCs detected at concentrations that met or exceeded human-health benchmarks in samples by well type, sampling region, and land use in the Long Island-New Jersey Study Unit.

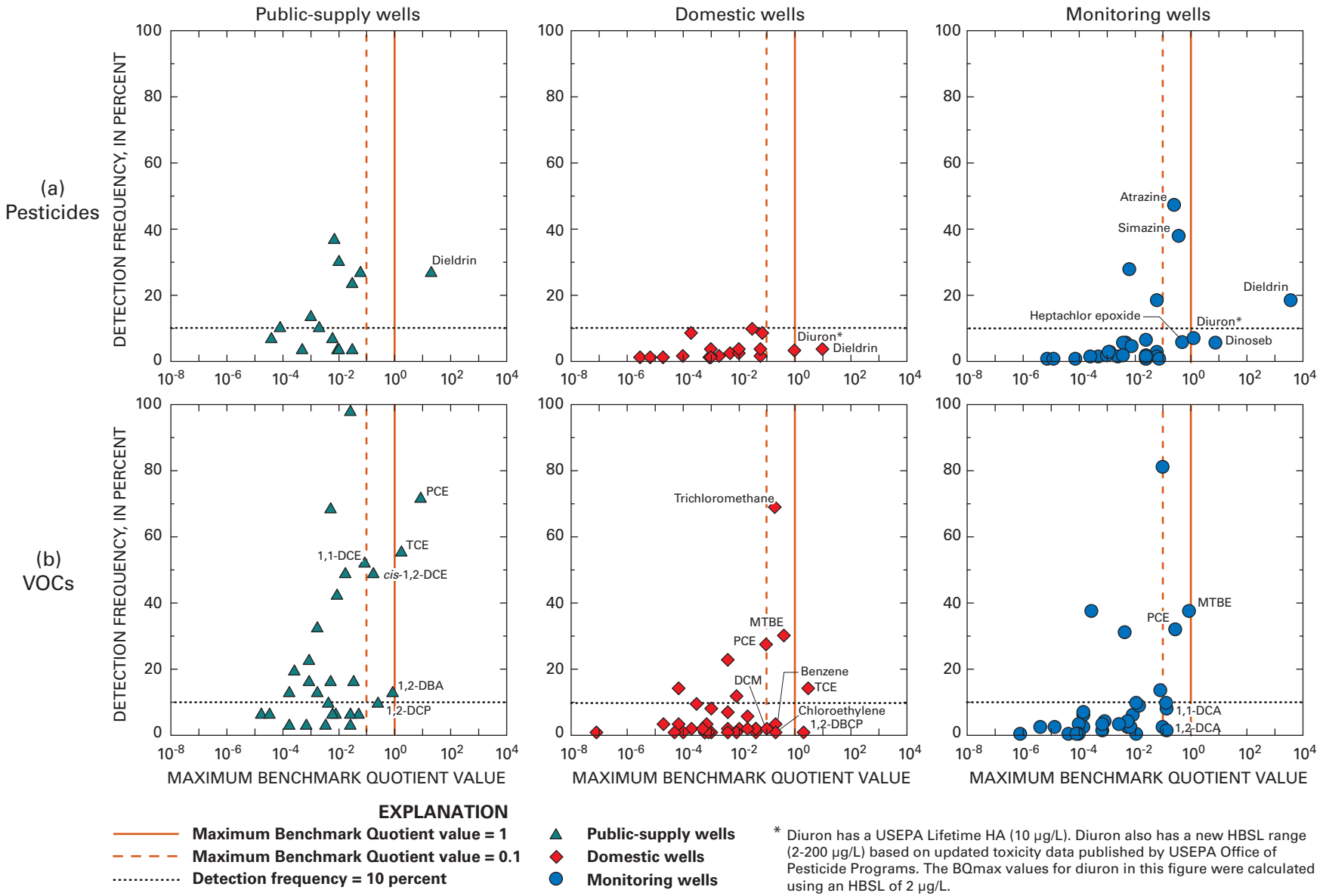
[Domestic-well data are presented by sampling region; monitoring-well data are presented by land-use category; VOC, volatile organic compound; **Bold type** indicates BQmax ≥ 1; BQmax, Benchmark Quotient = ratio of maximum detected concentration to human-health benchmark value; n, number of wells sampled; %, percent; PCE, tetrachloroethylene; TCE, trichloroethylene; --, not applicable; NA, not analyzed; µg/L, micrograms per liter; HBSL, Health-Based Screening Level; U.S. Environmental Protection Agency; MCL, Maximum Contaminant Level]

Well type	Sampling region	Land use and n wells	% Detected	Pesticides			VOCs			
			% Met or exceeded human-health benchmark	Dieldrin	Dinoseb	Diuron	1,2-Dibromo-3-chloropropane	1,2-Dibromo-ethane	PCE	TCE
Public-supply wells	Kirkwood-Cohansey Aquifer System	--	% Detected	26.7	NA	NA	0	13.3	73.3	56.7
		n=30	% BQmax ≥1	**23.3**	NA	NA	0	**3.3**	**3.3**	**3.3**
Domestic wells	Kirkwood-Cohansey Aquifer System	--	% Detected	0	0	6.7	3.3	0	30	16.7
		n=30	% BQmax ≥1	0	0	[1]**3.3**	**3.3**	0	0	0
	New England Physiographic Province	--	% Detected	3.3	0	0	0	0	30	10
		n=30	% BQmax ≥1	**3.3**	0	0	0	0	0	0
	Piedmont Physiographic Province	--	% Detected	9.5	NA	NA	0	0	18.2	18.2
		n=22	% BQmax ≥1	**9.5**	NA	NA	0	0	0	[2]**4.5**
Shallow monitoring wells	Kirkwood-Cohansey Aquifer System	Agricultural n=15	% Detected	6.7	20	13.3	0	0	6.7	13.3
			% BQmax ≥1	**6.7**	**13.3**	0	0	0	0	0
		New urban n=30	% Detected	26.7	0	0	0	0	30	6.7
			% BQmax ≥1	**26.7**	0	0	0	0	0	0
		Old urban n=20	% Detected	15	[3]0	[3]21.4	0	0	40	5
			% BQmax ≥1	10	[3]0	[3]**7.1**	0	0	0	0
		Undeveloped n=13	% Detected	0	7.7	0	0	0	15.4	0
			% BQmax ≥1	0	0	0	0	0	0	0
Moderate-depth monitoring wells	Kirkwood-Cohansey Aquifer System	New urban n=14	% Detected	21.4	NA	NA	0	0	42.9	7.1
			% BQmax ≥1	**21.4**	NA	NA	0	0	0	0
		Old urban n=16	% Detected	31.2	NA	NA	0	0	56.2	31.2
			% BQmax ≥1	**31.2**	NA	NA	0	0	0	0

[1]BQmax = 1 for diuron in Kirkwood-Cohansey aquifer domestic wells; diuron was detected at a concentration of 1.9 µg/L, nearly equal to the low end of its HBSL range (2 µg/L).

[2]TCE exceeded USEPA MCL (5 µg/L) 4.5% of the time and New Jersey MCL (1 µg/L) 9.1% of the time in domestic wells in the Piedmont Physiographic Province.

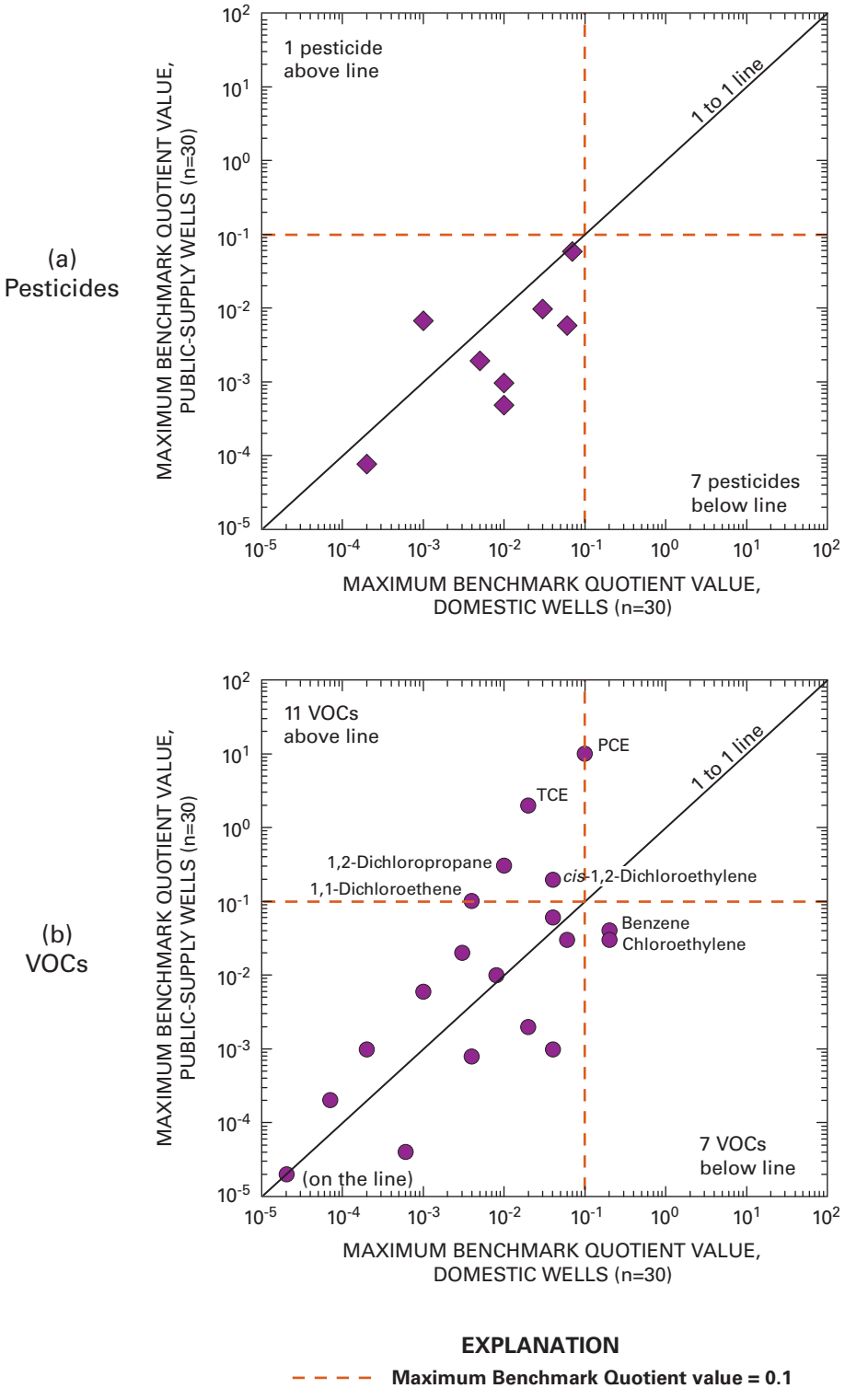
[3]n =14 for dinoseb and diuron in old urban shallow monitoring wells.



* Diuron has a USEPA Lifetime HA (10 µg/L). Diuron also has a new HBSL range (2-200 µg/L) based on updated toxicity data published by USEPA Office of Pesticide Programs. The BQmax values for diuron in this figure were calculated using an HBSL of 2 µg/L.

[BQmax, Maximum Benchmark Quotient = ratio of maximum detected concentration to human-health benchmark value; VOC, volatile organic compound; compounds with BQmax values ≥ 0.1 are labeled; ≥, greater than or equal to; 1,2-DBCP, 1,2-dibromo-3-chloropropane; 1,2-DBA, 1,2-dibromoethane; 1,1-DCA, 1,1-dichloroethane; 1,2-DCA, 1,2-dichloroethane; 1,1-DCE, 1,1-dichloroethene; *cis*-1,2-DCE, *cis*-1,2-dichloroethylene; DCM, dichloromethane (methylene chloride); 1,2-DCP, 1,2-dichloropropane; MTBE, methyl *tert*-butyl ether; PCE, tetrachloroethylene; TCE, trichloroethylene; %, percent; USEPA, U.S. Environmental Protection Agency; Lifetime HA, Lifetime Health Advisory; µg/L, micrograms per liter; HBSL, Health-Based Screening Level]

Figure 8. Detection frequencies and Maximum Benchmark Quotient values for (a) pesticides and (b) VOCs detected in public-supply wells, domestic wells, and monitoring wells in the Long Island-New Jersey Study Unit.



[BQmax, Maximum Benchmark Quotient = ratio of maximum detected concentration to human-health benchmark value; VOC, volatile organic compound; compounds with BQmax values ≥0.1 are labeled; ≥, greater than or equal to; n, number of samples; PCE, tetrachloroethylene; TCE, trichlorethylene]

Figure 9. Relation between Maximum Benchmark Quotient values for (a) pesticides and (b) VOCs detected in public-supply wells and those in domestic wells in the Kirkwood-Cohansey aquifer system, New Jersey.

Occurrence by Aquifer

Ground-water samples were collected from domestic wells in three aquifers (sampling regions) (figs. 1 and 2b). In samples from domestic wells, two pesticides (dieldrin, diuron) and two VOCs (1,2-dibromo-3-chloropropane and TCE) were present at maximum detected concentrations that met or exceeded human-health benchmarks (figs. 8a and 8b). Detection frequency and exceedance data for these four contaminants are listed by domestic-well sampling region in table 9.

Measured concentrations of dieldrin exceeded the low end of the HBSL concentration range in every sample from the New England and Piedmont Physiographic Provinces in which it was detected; dieldrin was not detected in domestic wells in the Kirkwood-Cohansey aquifer system. The measured concentration of diuron was approximately equal to the low end of the HBSL concentration range in one domestic-well sample from the Kirkwood-Cohansey aquifer system; diuron was not detected in the New England Physiographic Province and was not analyzed in samples from the Piedmont Physiographic Province (table 9). 1,2-Dibromo-3-chloropropane was detected and exceeded the USEPA and New Jersey MCL value in one of the 30 domestic-well samples from the Kirkwood-Cohansey aquifer system, but was not detected in samples from the New England or Piedmont Physiographic Provinces (table 9). TCE was frequently detected in all three domestic-well sampling regions, and measured concentrations exceeded the MCL value in two of the four samples from the Piedmont Physiographic Province in which it was detected (table 9).

Occurrence by Land Use

Ground-water samples were collected from shallow monitoring wells in four land-use areas (agricultural, new urban, old urban, and undeveloped areas) (fig. 2a) to measure the effects of land-use settings on shallow ground-water quality. In samples from monitoring wells, three pesticides (dieldrin, dinoseb, and diuron) but no VOCs had maximum detected concentrations that met or exceeded human-health benchmarks (figs. 8a and 8b). Detection frequency and exceedance data for these three pesticides are listed by land-use area in table 9.

Dieldrin, dinoseb, and diuron were detected in shallow monitoring wells in the agricultural land-use areas. These three pesticides were detected least often in shallow monitoring-well samples from undeveloped areas, and no concentrations detected from that land use met or exceeded human-health benchmarks. Dieldrin was detected in samples collected from all land-use categories, except undeveloped areas. Measured dieldrin concentrations met or exceeded human-health benchmarks in all but 1 of 12 shallow monitoring-well samples in which it was detected and in all of the moderate-depth monitoring wells in which it was detected (table 9; fig. 4), making dieldrin a compound of regional importance. Dinoseb was detected in samples collected from agricultural and undeveloped land-use areas, and measured concentrations exceeded the MCL in two of the three samples from agricultural land-use areas in which it was detected. Diuron was detected in samples collected in agricultural and old urban land-use areas, and the measured concentration was equal to the low end of the HBSL range in one of the three samples from the old urban land-use areas in which it was detected (table 9; fig. 4).

All the exceedances of human-health benchmarks in shallow monitoring wells were the result of pesticide detections in samples from the agricultural, old urban, and new urban land-use areas (table 9). The total number of pesticides and VOCs with BQmax values ≥ 0.1 was comparable for the agricultural (4), old urban (5), and new urban (3) land-use areas (data not shown). The fewest number of pesticides (8) and VOCs (9) were detected in samples from undeveloped land-use areas, as would be expected, and no pesticides or VOCs in the undeveloped land-use areas were detected within a factor of 10 of their human-health benchmarks (data not shown). Shallow monitoring wells were designed to sample parts of shallow aquifers that are known or suspected to be associated with specific land uses in the recharge area. Therefore, carefully located monitoring wells can provide an important indication of contamination in targeted parts of a ground-water flow system. Contamination detected in these monitoring wells can be both a contributor to, and a predictor of, future chemical contamination in deeper parts of the Kirkwood-Cohansey aquifer system, which is used for domestic and public supplies.

Contaminant Sources and Physicochemical Properties

Characterization of the sources and physicochemical properties of contaminants of potential human-health concern aids in understanding potential human exposure to these contaminants. The sources and physicochemical properties of contaminants that were frequently detected in the study unit were described in detail in another report (Stackelberg and others, 2000), but pertinent data related to the 20 contaminants of potential human-health concern are provided below.

Patterns of Occurrence of the Contaminants of Potential Human-Health Concern

When the 20 contaminants of potential human-health concern were examined in light of the five factors discussed above, the following four patterns of occurrence for these 20 contaminants emerged.

1. BQmax greater than or equal to 1, and frequently detected.
2. BQmax greater than or equal to 1, and not frequently detected.
3. BQmax less than 1 but greater than or equal to 0.1, and frequently detected.
4. BQmax less than 1 but greater than or equal to 0.1, and not frequently detected.

The occurrence of the contaminants that follow these four patterns is summarized below.

Pattern 1: BQmax Greater than or Equal to 1 and Frequently Detected

One unregulated pesticide (dieldrin) and three regulated VOCs (PCE, TCE, and 1,2-dibromoethane) were measured at concentrations that exceeded human-health benchmarks and were frequently detected in ground water that is used for drinking water (that is, domestic or public-supply wells) (table 8; figs. 6 and 7).

Dieldrin stands out because (1) it was measured at concentrations that exceeded the low end of the HBSL concentration range (10^{-6} cancer risk) in samples from all well types and (2) it was frequently detected in public-supply and monitoring wells (tables 4 and 8; fig. 6). Measured concentrations of dieldrin met or exceeded the low end of the HBSL concentration range in 29 of 31 samples in which it was detected (figs. 4 and 6), resulting in BQmed-det values that were ≥ 1 for all well types (table 8). Dieldrin was detected at concentrations within a factor of 10 of the HBSL in the two samples in which detected concentrations did not exceed the low end of the HBSL concentration range (figs. 4 and 6). Environmental residues of dieldrin may result from the introduction of either dieldrin or aldrin into the environment. Dieldrin and aldrin are organochlorine insecticides, which is a highly persistent class of insecticides used extensively in the United States during the 1950s-1960s; dieldrin also is a degradation product formed from aldrin. Both dieldrin and aldrin are no longer registered for use in the United States (Ware, 1989). Their uses were discontinued for agriculture in the early 1970s and for termite control in the late 1980s (Nowell and others, 1999).

Two VOCs (PCE and TCE) stand out because they were (1) detected at concentrations that exceeded their human-health benchmarks (USEPA and New Jersey MCLs) and (2) frequently detected in multiple well types. BQmed-det values for PCE and TCE were less than 0.1 for all well types (table 8), indicating that although these contaminants were frequently detected, they were not frequently detected at concentrations approaching MCL values.

PCE concentrations exceeded human-health benchmarks in only 1 of 30 public-supply well samples, but maximum detected concentrations were within a factor of 10 of human-health benchmarks in domestic and monitoring wells (tables 6 and 8; figs. 5 and 7). Unlike many of the VOCs of potential human-health concern, PCE is less soluble and more likely to sorb to organic matter in the subsurface than other chlorinated compounds (Stackelberg and others, 2000). Nonetheless, PCE was frequently detected in all well types, and in all sampling regions and land-use areas, with the exception of monitoring wells in agricultural land-use areas (table 9), reflecting its high-volume production and diverse industrial and commercial uses (Harte and others, 1991; Stackelberg and others, 2000).

TCE was measured in samples from public-supply and domestic wells at concentrations that exceeded its human-health benchmarks; it also was frequently detected in all well types (tables 6 and 8; figs. 5 and 7). TCE concentrations exceeded the USEPA MCL value in 1 of 30 samples from public-supply wells and 1 of 82 samples from domestic wells, and exceeded the New Jersey MCL value in 2 public-supply wells and 2 domestic wells (fig. 5). TCE was detected at concentrations within a factor of 10 of the New Jersey MCL in both shallow and moderate-depth monitoring wells (data not shown). TCE has been produced in large quantities since the 1960s and has a wide variety of industrial and commercial uses as a metal degreaser and industrial solvent, among other uses (Harte and others, 1991). TCE is likely to leach to ground water because it is highly water soluble and has a low soil-sorption coefficient (Stackelberg and others, 2000).

1,2-Dibromoethane was detected at concentrations that exceeded its human-health benchmarks (USEPA and New Jersey MCL values), and it was frequently detected, but only in samples from public-supply wells. 1,2-Dibromoethane was detected in 4 of 30 public-supply-well samples; only one sample had measured concentrations that exceeded the MCL, and this was an estimated concentration (tables 6 and 8; figs. 5 and 7). The other three detections were within a factor of 10 of the MCL (fig. 7). The occurrence of 1,2-dibromoethane exclusively in samples from the public-supply wells likely reflects historical use patterns and the fact that public-supply wells intercept ground water from larger contributing areas than other well types (Stackelberg and others, 2000). The analytical MRL for 1,2-dibromoethane in shallow monitoring wells was about 3-fold greater than that for the other well types (table 1), which may explain why it was not detected in shallow monitoring wells. 1,2-Dibromoethane was used historically as an additive to leaded gasoline and as a turf fumigant (U.S. Environmental Protection Agency, 2002f), but use of 1,2-dibromoethane has decreased with the decline in the use of leaded gasoline and because the USEPA banned its use as a turf fumigant in 1984 (Stackelberg and others, 2000).

Pattern 2: BQmax Greater than or Equal to 1 and not Frequently Detected

One regulated pesticide (dinoseb), one unregulated pesticide (diuron), and one regulated VOC (1,2-dibromo-3-chloropropane) were measured in samples at concentrations that exceeded human-health benchmarks in one or more well types, but were not frequently detected in any well type (table 8; figs. 6 and 7). Neither dinoseb nor diuron were analyzed in samples from public-supply wells, domestic wells from the Piedmont Physiographic Province, or moderate-depth monitoring wells (table 9).

The USEPA and New Jersey MCL value for dinoseb, a regulated pesticide, was met or exceeded (BQmax = 6) in two of the four monitoring-well samples in which it was detected, and detected concentrations of dinoseb were at least 100-fold less than the MCL in the other two samples (fig. 6). The MCL exceedances of dinoseb occurred in 2 of 15 samples from shallow, agricultural monitoring wells (table 9). The BQmed-det value for monitoring wells was 0.6 (table 8), indicating that at least half of the detected dinoseb concentrations were within a

factor of 10 of the MCL. Dinoseb was not detected in domestic-well samples and was not analyzed in public-supply well samples (tables 8 and 9; figs. 4 and 6). Dinoseb has a high potential for movement in the environment because it is moderately soluble in water and does not sorb appreciably to soil particles (Vogue and others, 1994).

The maximum detected concentration of diuron was equal to the low end of the HBSL concentration range (BQmax = 1) in 1 of 14 samples from the old-urban monitoring wells, and its measured concentration was approximately equal to the low end of the HBSL concentration range in 1 of 30 domestic-well samples from the Kirkwood-Cohansey aquifer system (tables 8 and 9). The BQmed-det value for diuron in domestic wells was 0.5 (table 8), but this was a result of its low detection frequency in domestic wells (2 of 60 samples) (fig. 6). Diuron has a new HBSL range (2-200 µg/L) based on updated toxicity data published by USEPA OPP (U.S. Environmental Protection Agency, 2002c). Diuron also has a Lifetime HA value of 10 µg/L published by USEPA OW; this Lifetime HA value was not exceeded in any sample. Diuron has a moderate potential for movement in the environment because of its moderate water solubility and ability to sorb to soil particles (Vogue and others, 1994).

1,2-Dibromo-3-chloropropane was analyzed in all well types, but was detected in only 1 of 82 domestic-well samples (table 8; figs. 5 and 7), in a domestic well in the Kirkwood-Cohansey aquifer system (table 9). This one measured concentration exceeded the USEPA and New Jersey MCL value for 1,2-dibromo-3-chloropropane (BQmax = 2), and because 1,2-dibromo-3-chloropropane was detected in only one sample, the BQmed-det value is the same as its BQmax value (table 8). Because 1,2-dibromo-3-chloropropane was detected in only one domestic well sample and was not detected in any of the other well types, it could be a compound of local, but probably not regional, importance. The low detection frequency of 1,2-dibromo-3-chloropropane, however, could be the result of its relatively high MRL value (0.214 µg/L) compared to other regulated VOCs (table 6). The MRL value is greater than the MCL for 1,2-dibromo-3-chloropropane (0.2 µg/L) in all well types (table 1). As a result, it is possible that this contaminant may be present, but undetected, at concentrations greater than the MCL but less the MRL, which means that the MCL exceedance rates could be biased low. 1,2-Dibromo-3-chloropropane is a fumigant with a very high potential for movement in the environment because it has high water solubility and limited ability to sorb to soil particles (Vogue and others, 1994).

Pattern 3: BQmax Less than 1 but Greater than or Equal to 0.1 and Frequently Detected

Two regulated pesticides (atrazine and simazine) and seven regulated VOCs (benzene, 1,1-dichloroethane, 1,1-dichloroethene, *cis*-1,2-dichloroethylene, 1,2-dichloropropane, MTBE, and trichloromethane) were measured at concentrations that did not exceed, but were within a factor of 10 of human-health benchmarks ($1 > BQmax \geq 0.1$) in one or more well types; they also were frequently detected in ground water that is used for drinking water (that is, domestic and (or) public-supply wells) (table 8; figs. 6 and 7). All nine contaminants had BQmed-det values of 0.04 or less for all well types (table 8), indicating that the median detected concentrations were at least a factor of 20 less than the USEPA or New Jersey MCL values.

Atrazine and simazine had BQmax values ≥ 0.1 but less than 1 only for monitoring-well samples (table 8; fig. 6) (that is, in water that is not immediately consumed as drinking water). Atrazine and simazine are high-use herbicides that are highly mobile because they are water soluble and do not sorb appreciably to soil particles (Stackelberg and others, 2000). Both atrazine and simazine were frequently detected in public-supply wells (table 4) and shallow and moderate-depth monitoring wells (data not shown).

Of the seven frequently detected VOCs with BQmax values ≥ 0.1 but less than 1, only MTBE and trichloromethane (chloroform) were frequently detected in all well types (table 8; fig. 7), indicating widespread (nonpoint) sources of these contaminants. MTBE was first used to enhance octane levels in gasoline in the late 1970s. By the early 1990s, MTBE became the most commonly used fuel oxygenate in many parts of the Nation (Zogorski and others, 1997). MTBE is more soluble, slower to degrade, and more mobile in the subsurface than other gasoline constituents such as benzene (Squillace and others, 1997). Trichloromethane is used in the production of fluorocarbon-22, but it also is a common disinfection byproduct resulting from the chlorination of public drinking-water supplies. These public supplies can provide widespread (nonpoint-source) recharge to surficial aquifers underlying urban areas through a variety of mechanisms (Stackelberg and others, 2000).

The remaining five frequently detected VOCs with BQmax values ≥ 0.1 but less than 1 are benzene and four chlorinated organic compounds (1,1-dichloroethane, 1,1-dichloroethene, *cis*-1,2-dichloroethylene, and 1,2-dichloropropane) (table 8; fig. 7). Benzene was frequently detected in public-supply wells (table 6) and moderate-depth monitoring wells (data not shown). Benzene is used as a constituent in motor fuels, as a solvent for a variety of media, and in the manufacture of detergents, explosives, pharmaceuticals, and dyestuffs (U.S. Environmental Protection Agency, 2002f). The four chlorinated organic compounds were frequently detected in public-supply wells (table 6); 1,1-dichloroethane and 1,1-dichloroethene also were frequently detected in moderate-depth monitoring wells (data not shown). These four chlorinated compounds are used in industrial and commercial applications similar to those of PCE and TCE, although in much smaller quantities (Stackelberg and others, 2000). These four chlorinated compounds have moderate to high water solubilities and low soil-sorption coefficients, indicating that they likely leach to ground water after being introduced to the subsurface (Stackelberg and others, 2000).

Pattern 4: BQmax Less than 1 but Greater than or Equal to 0.1 and not Frequently Detected

One regulated pesticide (heptachlor epoxide) and three regulated VOCs (chloroethylene, 1,2-dichloroethane, and methylene chloride) were measured at concentrations that did not exceed, but were within a factor of 10 of human-health benchmarks ($1 > BQmax \geq 0.1$) in one or more well types, but were not frequently detected in any well type (table 8; figs. 6 and 7).

Heptachlor epoxide was analyzed only in shallow monitoring-well samples. Heptachlor epoxide had a BQmax value of 0.4 in these samples, where it was detected infrequently (4 out of 69 samples) (table 8; fig. 6). The BQmed-det value for heptachlor epoxide is 0.1 (table 8), indicating that the median detected concentration was a factor of 10 less than the USEPA MCL. Heptachlor epoxide is a persistent degradation product of the organochlorine insecticide heptachlor (U.S. Environmental Protection Agency, 2002e), which is no longer used in the United States. Heptachlor was used widely to control fire ants in the Southeast and as a soil insecticide on corn and other food crops until the mid-1970s, and was used in termite control until the late 1980s (Nowell and others, 1999).

Chloroethylene was detected infrequently in public-supply and domestic wells, and its BQmax value was 0.2 for domestic wells. Chloroethylene was detected in only 1 of 82 domestic-well samples; hence, its BQmed-det value for domestic wells was the same as its BQmax value (table 8). 1,2-Dichloroethane was detected infrequently in all three well types, and its BQmax value was 0.1 for monitoring-well samples. Methylene chloride was found only in domestic wells, where it was detected in 2 of 82 domestic-well samples; the BQmax value was 0.1. The BQmed-det value for methylene chloride also was 0.1 because both detections of methylene chloride were within a factor of 10 of the USEPA MCL (table 8; fig. 7). These three chlorinated solvents typically are used in organic synthesis or as solvents and have limited ability to sorb to soil particles due to low soil-sorption coefficients (Mackay and others, 1993).

In addition to the 20 contaminants of potential human-health concern described above, one additional contaminant, deethylatrazine, is noteworthy because it was frequently detected in all well types, but it has no human-health benchmarks. This contaminant is formed in the environment from degradation of the commonly used herbicides atrazine and propazine, which makes deethylatrazine a high priority for the collection of toxicity information. In the USEPA OPP Human-Health Risk Assessment for atrazine, the toxicity of deethylatrazine was considered as equivalent to that of the parent compound atrazine (U.S. Environmental Protection Agency, 2002d). The consensus-based protocol for HBSL development (Toccalino and others, 2003), however, does not currently permit the use of toxicity data from a parent compound to calculate an HBSL for a degradation product; the HBSL protocol is based on USEPA OW methodologies.

Health-Based Comparison of Wells with Multiple Contaminants

A major objective of this pilot effort is to demonstrate use of the HBSL approach as a tool for communicating water-quality data collected for individual contaminants in a human-health context. Guidance for interpreting water-quality data for multiple contaminants in a human-health context is not provided in the "Guidance" section of this report because such interpretations represent an extension beyond typical analyses. Additionally, USEPA procedures for assessing potential risks or hazards resulting from exposure to multiple contaminants are under development (Toccalino and others, 2003). Nonetheless, an initial effort was made to communicate water-quality findings for multiple contaminants in a human-health context because multiple chemicals (53 in public-supply, 68 in domestic, and 75 in monitoring wells) were detected in each type of well (table 3). In this section, a screening tool for interpreting the occurrence of multiple contaminants in a human-health context is presented as a first step towards estimating relative potential human-health concerns associated with individual wells.

The long-term cumulative effects of low concentrations of multiple contaminants on human health currently are unknown and are an area of active research. Early USEPA guidance on the assessment of chemical mixtures indicated that when toxicity data are not available for an identical or reasonably similar mixture to that being studied, the risk or hazard can be estimated from the toxic or carcinogenic properties of the components in the mixture. When little or no quantitative information is available on the potential interactions between the components in a mixture, additive models are recommended (U.S. Environmental Protection Agency, 1986, 1989b). As these early guidance documents note, however, dose-additive models are not the most biologically plausible approach if the compounds do not have the same mode of toxicological action; more recent USEPA guidance documents have begun to address this issue (U.S. Environmental Protection Agency, 2000, 2002a, 2003d). The approach used in this report does not make assumptions about dose additivity or modes of toxicological action.

Mixtures of contaminants were detected in each of the well types considered in this study. Previous analyses examined the co-occurrence of pesticides and VOCs in public-supply and monitoring wells in the Kirkwood-Cohansey aquifer system (Stackelberg and others, 2001). One or more pesticides were detected with one or more VOCs in more than 95 percent of the samples collected from these well types. Overall, more than 140,000 and more than 3,000 unique combinations of pesticides with VOCs were detected in two or more samples from the public-supply and monitoring wells, respectively. The most frequently detected pesticides (such as atrazine, simazine, deethylatrazine) and VOCs (such as trichloromethane and MTBE) constituted the most frequently occurring combinations (Stackelberg and others, 2001).

Benchmark Quotient Computations for Multiple Contaminants in Individual Wells

Two BQ indexes were computed to aid in the examination of the occurrence of multiple contaminants in individual wells in relation to their respective human-health benchmarks. To ensure comparability between BQ calculations for different well types, aquifers (sampling regions), and land-use areas, only the 47 pesticides and 85 VOCs that were analyzed in all well types were considered in the analyses; of these, 44 pesticides and 55 VOCs have human-health benchmarks. Water-quality data from 30 public-supply, 82 domestic, and 108 monitoring wells were evaluated. At least one pesticide or VOC with a human-health benchmark was detected in most individual wells (100 percent of public-supply wells, 88 percent of domestic wells, and 98 percent of monitoring wells) (table 10). The maximum numbers of pesticides and VOCs with human-health benchmarks that were detected in any individual well were 21 for public-supply wells, 24 for domestic wells, and 17 for monitoring wells (table 10).

For each individual well, BQ values were calculated for every detected compound with a human-health benchmark, and these BQ values were used to determine two BQ indexes for that well—the maximum BQ value (BQSiteMax) and the sum of all BQ values (BQSiteSum). (Computations are shown for a hypothetical example in table 11.) **BQSiteMax** is defined as the maximum of BQ values for all detected contaminants in a given well. BQSiteMax will be greater than or equal to 1 if measured concentrations of any contaminant in the sample exceed or are equal to the human-health benchmark.

BQSiteSum is defined as the sum of all BQ values for a given well. In other words, BQSiteSum is a unitless sum of the concentrations of individual contaminants in a mixture, with each concentration first normalized by dividing the concentration by its respective human-health benchmark; each contaminant with a human-health benchmark is weighted equally. The BQSiteSum provides a relative measure of potential for human-health effects for individual wells and, therefore, is appropriate and valuable to use as a screening-level tool in water-quality analyses. For example, BQSiteSum values can be used to compare and rank wells, or well types, on the basis of relative potential human-health concerns to help prioritize future sampling efforts. Also, BQSiteSum values observed over time in individual wells can be used to track trends in potential for human-health effects.

Because BQSiteSum values provide a relative measure of potential human-health effects in individual wells, the biological importance of any absolute BQSiteSum value is unknown. A BQSiteSum value ≥ 1 does not necessarily indicate an exceedance of any human-health standard or guideline, unless measured concentrations of one or more individual compounds in a sample exceed their respective human-health benchmarks. For example, if 10 compounds are measured at concentrations within a factor of 10 of their respective human-health benchmarks in a given well and the BQSiteSum value is ≥ 1, this does not necessarily indicate that there is a potential for adverse health effects.

BQSiteSum values are analogous to the Pesticide Toxicity Index, which can be used to rank sites on the basis of relative potential exposure and toxicity of pesticides to aquatic organisms (Munn and Gilliom, 2001). BQSiteSum values also are similar to Hazard Index (HI) values used by USEPA to assess noncancer hazards. HI values are the sum of more than one hazard quotient (HQ) for multiple substances and (or) multiple exposure pathways. An HQ is the ratio of a single substance exposure level to a reference dose toxicity value. If the HI is greater than 1 as a result of summing several HQs of similar magnitude, USEPA segregates the compounds by effects and by mechanism of action and then derives separate HIs for each chemical group (U.S. Environmental Protection Agency, 1989b). In contrast to HI values, BQSiteSum values do not distinguish between carcinogens and noncarcinogens or make assumptions about modes of toxicological action, nor do they imply that contaminant toxicities or carcinogenicities are additive.

Compounds without human-health benchmarks were excluded from the BQSiteMax and BQSiteSum calculations. In preliminary analyses (data not shown), BQ values for compounds that were not detected, but have human-health benchmarks, were calculated using two methods: (1) assume a concentration of zero, and (2) assume a concentration equal to the MRL. These preliminary analyses showed that the treatment of nondetects generally had little influence on the results except for BQ values calculated for compounds that have MRL values near or greater than their MCL or HBSL value; these BQ values artificially inflated BQSiteSum values. Therefore, compounds that were not detected, but have human-health benchmarks, were assigned BQ values of zero (table 11).

Occurrence of Multiple Contaminants by Well Type

Cumulative distribution plots of BQSiteMax and BQSiteSum values for pesticide data, VOC data, and the combination of pesticide and VOC data for individual wells in all three well types are shown in figure 10. For most individual wells, BQSiteMax values were equivalent to, or close to, BQSiteSum values, particularly for pesticides. For pesticides, the median ratio of BQSiteMax to BQSiteSum values was approximately 1 for all well types; for VOCs, this median ratio ranged from 0.77 for public-supply wells to 0.94 for domestic wells (fig. 10), indicating that the BQSiteMax value makes up the majority of the sum. In all samples and for all analytes (pesticides, VOCs, and pesticides plus VOCs combined), the BQSiteMax value was within a factor of 10 of the BQSiteSum value.

For all well types, pesticides with human-health benchmarks were detected in fewer individual wells than were VOCs with human-health benchmarks (table 10; figs. 10a and 10b). More individual wells had detections of pesticides with BQSiteMax values ≥ 1 (28 of 219 wells), however, than had

Table 10. Numbers of (1) individual wells with contaminant detections and (2) compounds detected with human-health benchmarks in individual wells in the Long Island-New Jersey Study Unit.

[n, number of wells sampled; HH benchmark, Human-health benchmark (MCL or HBSL); %, percent; BQ, Benchmark Quotient = ratio of measured concentration to human-health benchmark value; BQSiteMax, maximum Benchmark Quotient value in an individual well; ≥, greater than or equal to; PSW, public-supply well; DW, domestic well; MW, monitoring well; VOC, volatile organic compound]

Well type	n	Number (%) of wells with detections of compounds with HH benchmarks		Maximum number of compounds detected with HH benchmarks in any well	Number (%) of wells with detections of compounds with BQSiteMax ≥1		Maximum number of compounds detected with BQ value ≥1 in any well	Number (%) of wells with detections of compounds with BQSiteMax ≥0.1		Maximum number of compounds detected with BQ value ≥0.1 in any well
Pesticides										
PSW	30	23	(77%)	6	7	(23%)	1	8	(27%)	1
DW	81	21	(26%)	5	3	(4%)	1	3	(4%)	1
MW	108	78	(72%)	11	18	(17%)	1	25	(23%)	2
VOCs										
PSW	30	30	(100%)	20	3	(10%)	1	12	(40%)	2
DW	82	69	(84%)	20	2	(2%)	1	8	(10%)	3
MW	108	101	(94%)	13	0	(0%)	0	5	(5%)	2
Pesticides and VOCs										
PSW	30	30	(100%)	21	9	(30%)	2	18	(60%)	3
DW	82	72	(88%)	24	5	(6%)	1	9	(11%)	3
MW	108	106	(98%)	17	19	(18%)	1	29	(27%)	2

detections of VOCs with BQSiteMax values ≥ 1 (5 of 220 wells) (table 10; figs. 10a and 10b). A BQSiteMax value ≥ 1 indicated that the maximum detected concentration of at least one contaminant in an individual well met or exceeded a human-health benchmark (MCL or HBSL value). For pesticides and VOCs combined, public-supply wells had the largest percentage of individual wells (9 of 30 or 30 percent) with a BQSiteMax value ≥ 1. The BQSiteMax value was ≥ 1 for 5 of 82 (6 percent) domestic wells and for 19 of 108 (18 percent) monitoring wells (table 10 and fig. 10c). In public-supply and domestic wells, pesticides contributed approximately two-thirds of the measured exceedances, whereas in monitoring wells, all exceedances resulted from measured pesticide concentrations (table 10). All BQSiteMax values ≥ 1 for pesticides resulted from dieldrin detections. Dinoseb and diuron also had BQ values ≥ 1 in domestic and (or) monitoring wells (fig. 6), but dinoseb and diuron were not analyzed in all well types. Because only contaminants analyzed in all well types are considered for this evaluation, dinoseb and diuron do not contribute to BQSiteMax or BQSite Sum values. BQSiteMax values ≥ 1 for VOCs resulted from exceedances in one public-supply well each for 1,2-dibromoethane, PCE, and TCE and one domestic well each for 1,2-dibromo-3-chloropropane and TCE (fig. 7). For all three well types, the greatest BQSiteMax and BQSite-Sum values (20, 10, and 3,000 for public-supply, domestic, and monitoring wells, respectively) were the result of pesticide (dieldrin) detections (figs. 6, 10a and 10c).

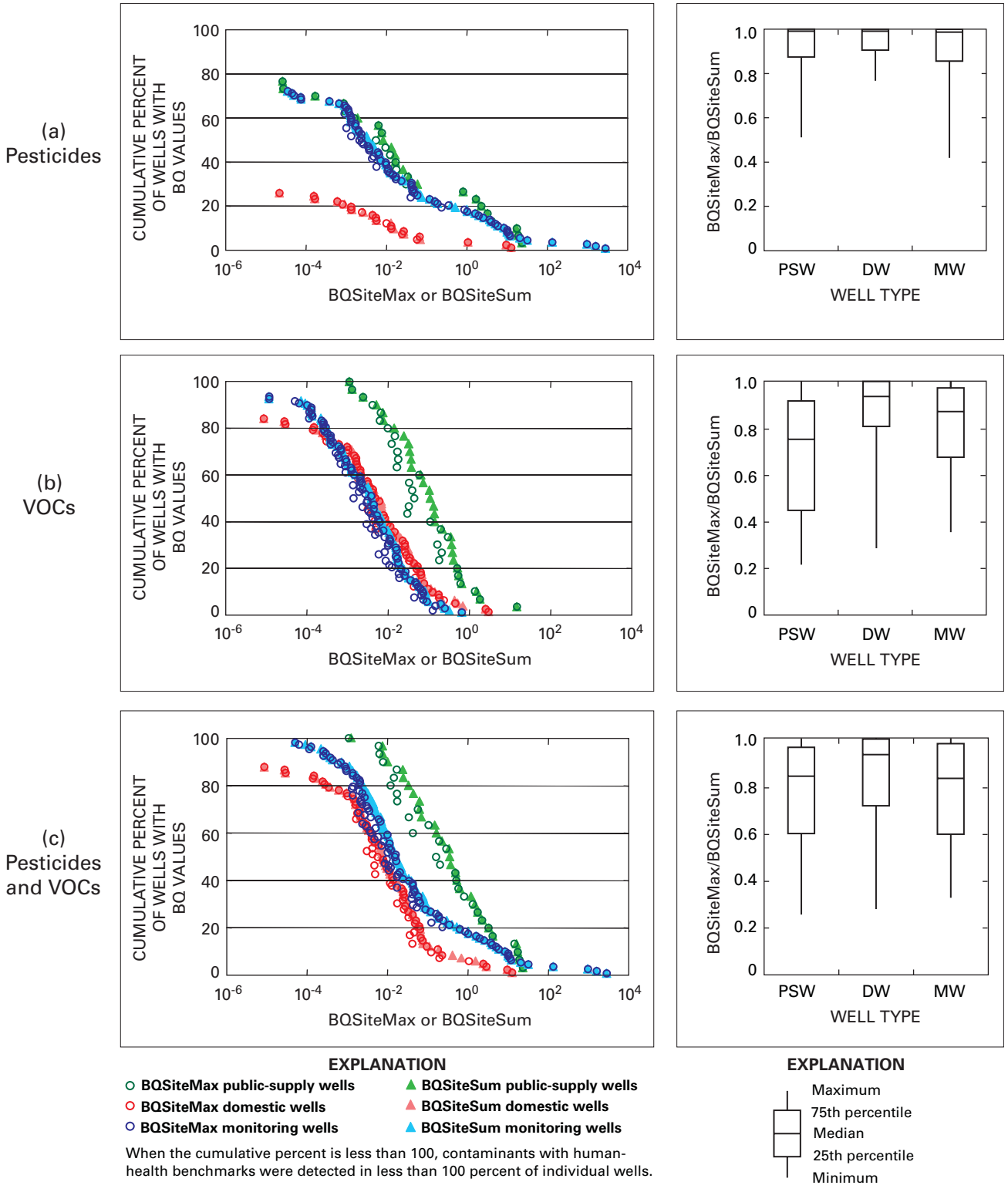
Results of analysis of variance on the ranked-transformed BQSiteMax values for pesticides and VOCs combined indicate that the BQSiteMax values were statistically different for samples from all three well types in the study area at a 95-percent confidence level. A comparison of the means of BQSiteMax values for each well type using the Tukey test indicates that BQSiteMax values for public-supply wells were significantly greater than those for domestic wells and monitoring wells at a 95-percent confidence level, likely because public-supply wells had the largest percentage (30 percent) of individual wells with pesticide or VOC concentrations that exceeded their human-health benchmarks. Results of these two statistical tests were the same using BQSiteSum values. Results for domestic wells may not be directly comparable to results for public-supply or monitoring wells because public-supply and monitoring-well samples are from the Kirkwood-Cohansey aquifer system only, whereas domestic-well samples are from three aquifers (the Kirkwood-Cohansey aquifer system and aquifers in the Piedmont and New England Physiographic Provinces) (see sections "Description of Study Area" and "Well Networks"). Although samples from public-supply wells tended to have greater BQSiteMax and BQSiteSum values than samples from monitoring wells, the five highest BQSiteMax values for pesticides, and for pesticides and VOCs combined, are for monitoring wells (fig. 10).

A comparison of the means of BQSiteMax and BQSite-Sum values for domestic and monitoring wells using the Tukey test indicates that BQ values for monitoring wells are significantly greater than those for domestic wells at a 95-percent confidence level. This result is expected because shallow monitoring wells were designed to intentionally sample specific points in a shallow aquifer that are known, or suspected, to be associated with a part of the ground-water flow system that has been affected by contaminant sources that can be linked to known surficial land uses (such as pesticides applied to an agricultural field) in the recharge area.

Table 11. Hypothetical BQSiteMax and BQSiteSum example calculations for three compounds in three wells.

[µg/L, micrograms per liter; HH Benchmark, Human-Health Benchmark (MCL or HBSL); MCL, Maximum Contaminant Level; HBSL, Health-Based Screening Level; BQ, Benchmark Quotient = ratio of measured concentration to human-health benchmark value; BQSiteMax, maximum Benchmark Quotient value in an individual well; BQSiteSum, sum of all Benchmark Quotient values in an individual well; µg/L, micrograms per liter; ND, not detected]

Well number	Compound 1			Compound 2			Compound 3			BQSiteMax	BQSiteSum (rounded to 1 significant figure)
	Measured concentration (µg/L)	HH benchmark (µg/L)	BQ	Measured concentration (µg/L)	HH benchmark (µg/L)	BQ	Measured concentration (µg/L)	HH benchmark (µg/L)	BQ		
1	0.06	2	0.03	0.03	3	0.01	0.08	40	0.002	0.03	0.04
2	ND	2	0	.06	3	.02	.02	40	.0005	.02	.02
3	ND	2	0	.006	3	.002	ND	40	0	.002	.002



[BQ, Benchmark Quotient = ratio of measured concentration to human-health benchmark value; VOC, volatile organic compound; BQSiteMax = maximum BQ value in an individual well; BQSiteSum, sum of all BQ values in an individual well; PSW, public-supply well; DW, domestic well; MW, monitoring well]

Figure 10. Cumulative distributions and ratios of maximum and summed Benchmark Quotient values for individual wells for (a) pesticides, (b) VOCs, and (c) pesticides and VOCs with human-health benchmarks detected in public-supply, domestic, and monitoring wells in the Long Island-New Jesey Study Unit.

Occurrence of Multiple Contaminants by Aquifer and Land Use

In this study, ground-water quality data were collected for multiple aquifers and land-use areas, in addition to multiple well types. Cumulative distribution plots of the domestic-well data, separated by aquifer, are presented in figure 11 for pesticide data, VOC data, and pesticide and VOC data combined. For pesticide and VOC data combined, 1 of 30 domestic wells in each of the Kirkwood-Cohansey aquifer system and the New England Physiographic Province had BQSiteMax values ≥ 1 (as a result of 1,2-dibromo-3-chloropropane and dieldrin exceedances, respectively), and 3 of 22 wells in the Piedmont Physiographic Province had BQSiteMax values ≥ 1 (as a result of two dieldrin and one TCE exceedances) (table 9; fig. 11). Results of analysis of variance on the ranked-transformed BQSiteMax values for pesticides and VOCs combined indicate that the BQSiteMax values were statistically similar for domestic-well samples from different aquifers (Kirkwood-Cohansey aquifer system and the New England and Piedmont Physiographic Provinces), at a 95-percent confidence level. Results of this statistical test were the same using BQSiteSum values.

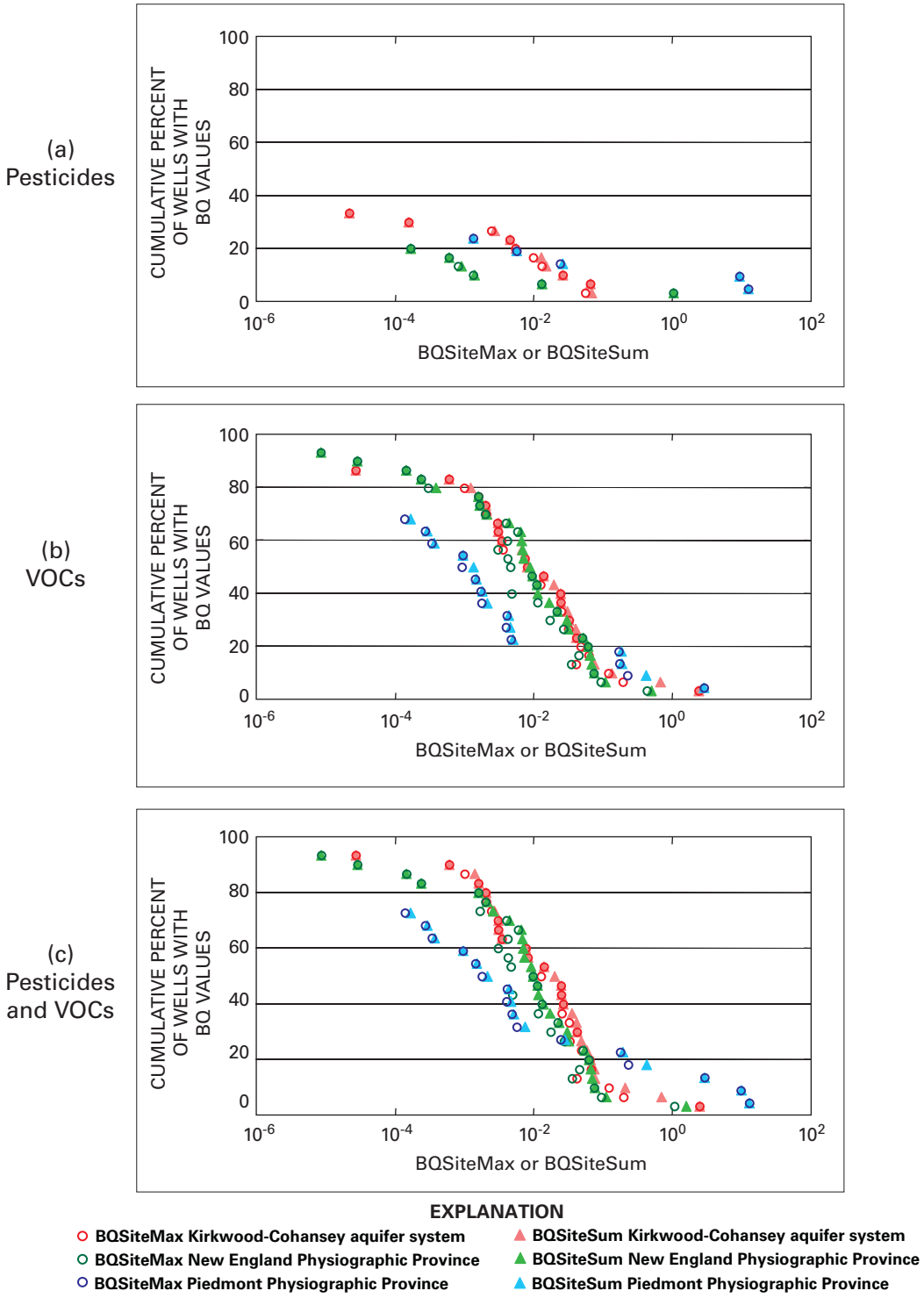
Cumulative distribution graphs of the shallow monitoring-well data, plotted as a function of land use, are presented for pesticide data (fig. 12a), VOC data (fig. 12b), and pesticide and VOC data combined (fig. 12c). Pesticides and VOCs with human-health benchmarks were detected in at least 70 percent of the individual shallow monitoring wells in most land uses (figs. 12a and 12b); the only exception is pesticides in shallow monitoring wells in the undeveloped land-use area (31 percent detection) (fig. 12a). No wells from the undeveloped land-use area had BQSiteMax or BQSiteSum values ≥ 1; the highest BQ value from an individual undeveloped land-use well was 0.02, a factor of 50 less than human-health benchmarks. No VOCs were detected at concentrations greater than human-health benchmarks in any of the individual shallow monitoring wells from any land-use area (fig. 12b). All of the exceedances of human-health benchmarks (that is, BQSiteMax ≥ 1) were the result of pesticide (dieldrin) detections in one agricultural well, two old-urban wells, and eight new-urban wells (table 9; figs. 12a and 12c).

Results of analysis of variance on the ranked-transformed BQSiteMax values for pesticides and VOCs combined indicate that the BQSiteMax values were statistically different for samples from shallow monitoring wells in different land-use areas (agricultural, old urban, new urban, and undeveloped), at a 95-percent confidence level. A comparison of the means of BQSiteMax values for each shallow monitoring well by land-use area using the Tukey test indicates that BQSiteMax values for wells in undeveloped land-use areas were significantly less than those for wells in new urban areas at a 95-percent confidence level. Results of these two statistical tests were the same using BQSiteSum values. Although figure 12c shows a pattern of consistently lower BQ values for shallow monitoring wells in the undeveloped land-use areas than those in other land-use areas, the Tukey test did not indicate that BQ values for wells in undeveloped areas were significantly different than for wells in agricultural or old urban areas at a 95-percent confidence level, perhaps because the sample sizes were too small to see significant differences between BQ values and because the distributions are similar.

Benefits of Applying Health-Based Screening Levels to Water-Quality Data

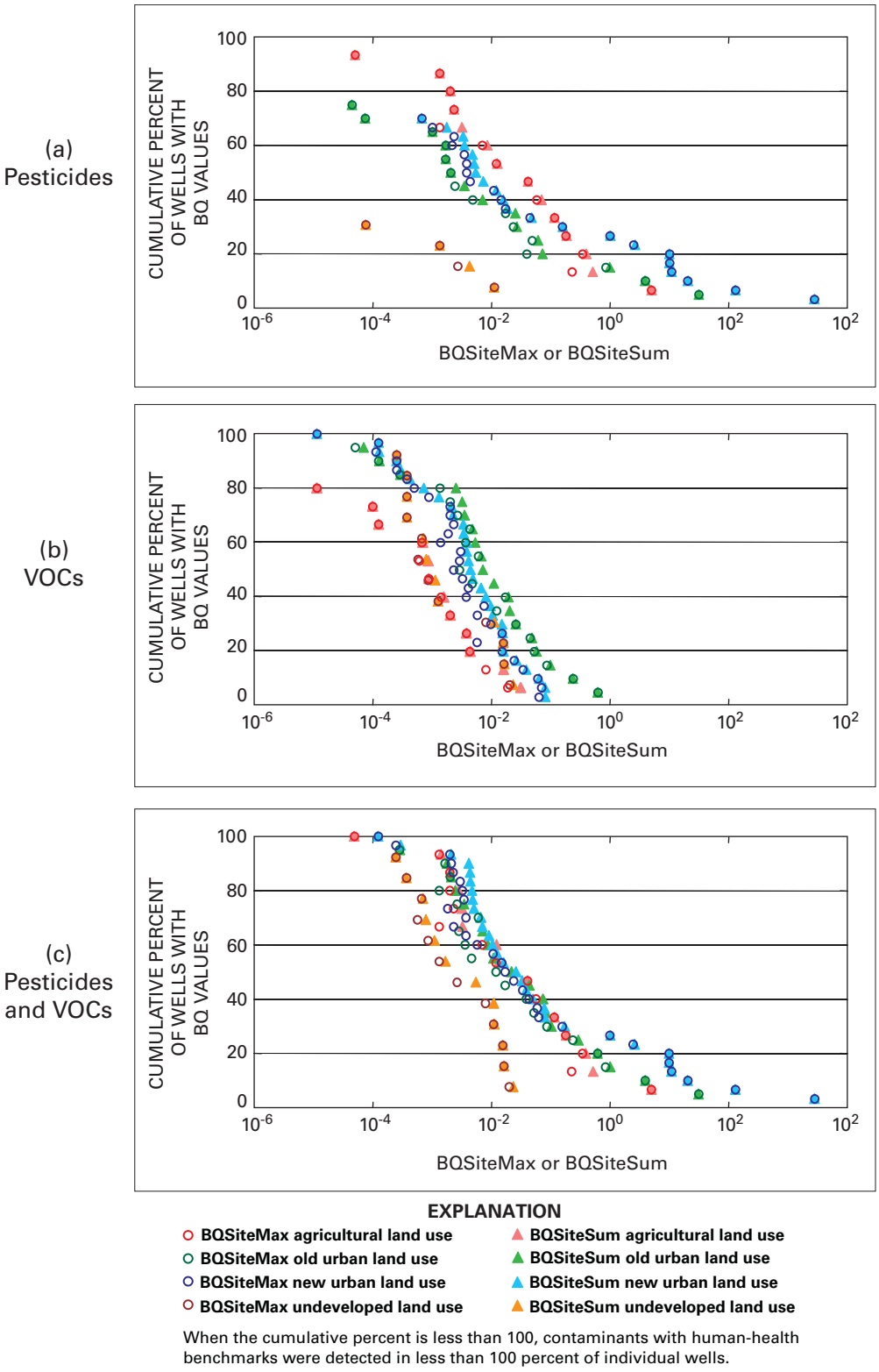
HBSL values increase the number of compounds with human-health benchmarks analyzed and detected in this study, thereby expanding the basis for interpreting contaminant-occurrence data in a human-health context. USEPA human-health benchmarks (that is, MCL, Lifetime HA, or RSD values) currently do not exist (as of August 2004) for 79 of the 182 compounds analyzed in this study. New HBSL values were calculated for 39 of these 79 unregulated compounds, plus an additional 7 compounds for which updated toxicity data were available. The 46 new HBSL values for 37 pesticides and 9 VOCs are provided in Appendix 2. New HBSL values increase the total number of analytes with human-health benchmarks from 103 of 182 compounds (57 percent) to 142 (78 percent) and the total number of detected compounds with human-health benchmarks from 65 of 97 compounds (67 percent) to 77 (79 percent). Acceptable USEPA toxicity values are not available for the remaining 40 (out of the 79) analytes without existing human-health benchmarks; therefore, HBSL values could not be determined for these 40 analytes (10 pesticides and 30 VOCs) (Appendix 3).

Fourteen of the 46 compounds with new HBSL values were detected in this study, increasing the total number of detected unregulated compounds with human-health benchmarks from 24 of 56 compounds (43 percent) to 36 (64 percent) (fig. 3). Two of the 14 detected unregulated compounds with new HBSL values (carbaryl and diuron) have Lifetime HA values published by USEPA OW, but new HBSL ranges were calculated using updated toxicity data published by USEPA OPP. The Lifetime HA values for carbaryl and diuron published in 1988 are based on their USEPA OW cancer classifications as Group D carcinogens, indicating that they are not classifiable as to human carcinogenicity (U.S. Environmental Protection Agency, 2004). More recent toxicity data published by USEPA OPP indicates that carbaryl and diuron are "likely to be carcinogenic to humans" and "known/likely" carcinogens, respectively (U.S. Environmental Protection Agency, 2002c and 2003e). For comparison purposes, the figures and tables in this report that include carbaryl and diuron provide both their HBSL concentration ranges and Lifetime HA values. Carbaryl was not identified as a contaminant of potential human-health concern in any well type. Diuron was identified as a contaminant of potential human-health concern in domestic and monitoring wells (BQmax = 1) using the low end of the HBSL range (tables 5 and 8), but it also would have been identified as a contaminant of potential human-health concern in these wells types using the Lifetime HA value (table 5).



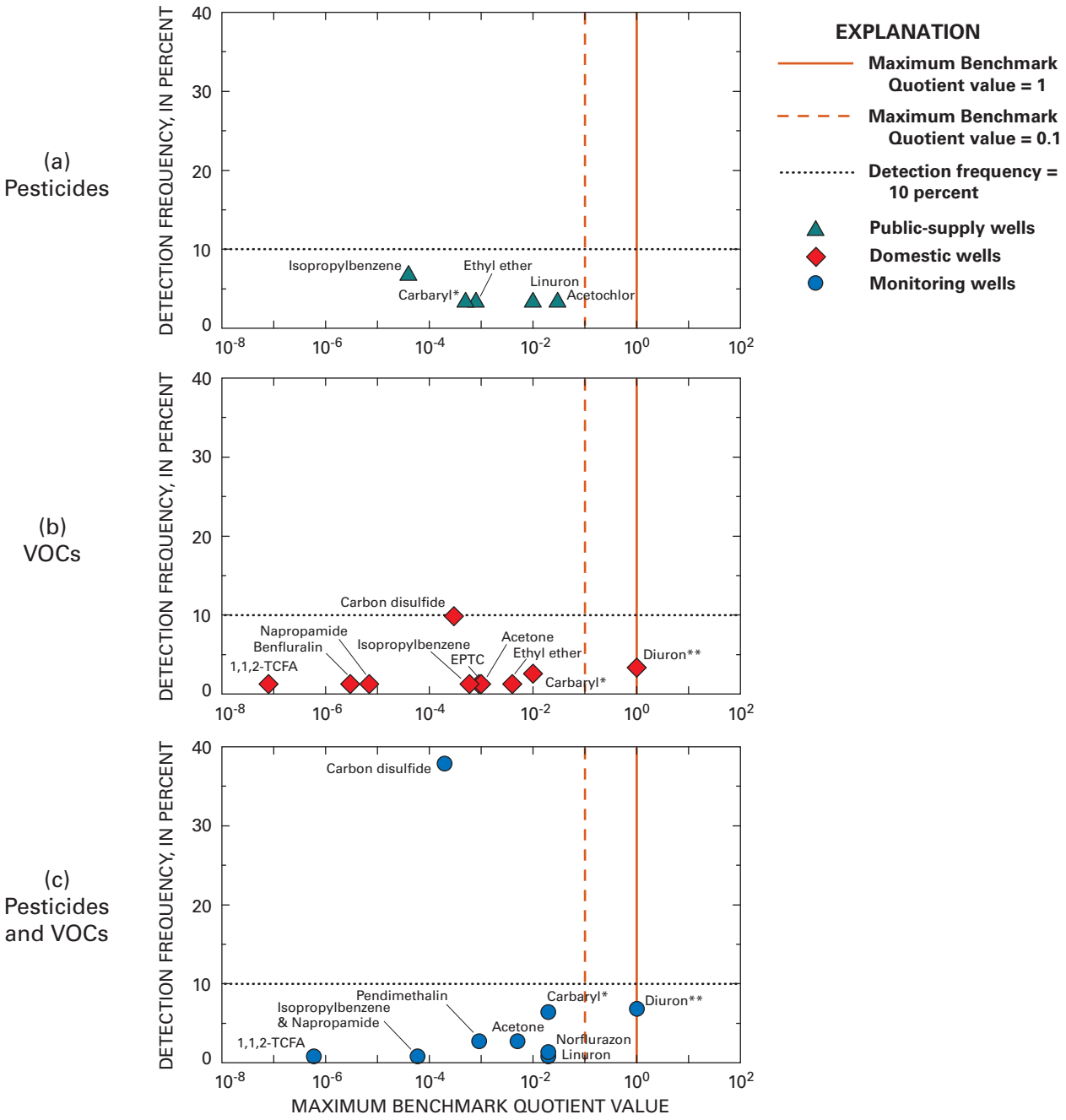
[BQ, Benchmark Quotient = ratio of measured concentration to human-health benchmark value; VOC, volatile organic compound; BQSiteMax = maximum BQ value in an individual well; BQSiteSum, sum of all BQ values in an individual well]

Figure 11. Cumulative distributions of Benchmark Quotient values for (a) pesticides, (b) VOCs, and (c) pesticides and VOCs with human-health benchmarks detected in individual domestic wells in the Kirkwood-Cohansey aquifer system, and aquifers in the New England and Piedmont Physiographic Provinces in the Long Island-New Jersey Study Unit.



[BQ, Benchmark Quotient = ratio of measured concentration to human-health benchmark value; VOC, volatile organic compound; BQSiteMax = maximum BQ value in an individual well; BQSiteSum, sum of all BQ values in an individual well]

Figure 12. Cumulative distributions of Benchmark Quotient values for (a) pesticides, (b) VOCs, and (c) pesticides and VOCs with human-health benchmarks detected in individual shallow monitoring wells representing agriculture, old urban, new urban, and undeveloped land uses in the Kirkwood-Cohansey aquifer system in the Long Island-New Jersey Study Unit.



* Carbaryl has a USEPA Lifetime HA value (700 µg/L); it also has a new HBSL range (40-4,000 µg/L) based on updated toxicity data published by USEPA Office of Pesticide Programs. BQmax values for carbaryl in this figure were calculated using an HBSL of 40 µg/L.

** Diuron has a USEPA Lifetime HA (10 µg/L). Diuron also has a new HBSL range (2-200 µg/L) based on updated toxicity data published by USEPA Office of Pesticide Programs. BQmax values for diuron in this figure were calculated using an HBSL of 2 µg/L.

[BQmax, Maximum Benchmark Quotient = ratio of maximum detected concentration to human-health benchmark value; VOC, volatile organic compound; HBSL, Health-Based Screening Level; 1,1,2-TCFA, 1,1,2-trichloro-1,2,2-trifluoroethane; EPTC, 5-ethyl dipropylthiocarbamate; USEPA, U.S. Environmental Protection Agency; Lifetime HA, Lifetime Health Advisory; µg/L, micrograms per liter]

Figure 13. Detection frequencies and Maximum Benchmark Quotient values for unregulated pesticides and VOCs with new HBSL values detected in (a) public-supply wells, (b) domestic wells, and (c) monitoring wells in the Long Island-New Jersey Study Unit.

The other 12 detected compounds that have new HBSL values were detected at concentrations ranging from 30- to 12-million-fold less than HBSL values (BQmax < 0.1) in all three well types (fig. 13) and, therefore, were not identified as being contaminants of potential human-health concern in any well type. Before HBSL values were calculated, these 12 compounds would have been detected, but their occurrence could not have been interpreted in a human-health context using USEPA drinking-water standards and guidelines. Twelve of the 14 detected unregulated compounds with new HBSL values were detected in public-supply and (or) domestic wells, and all but diuron have BQmax values less than 0.1 (fig. 13a and 13b). Because these water resources are used as drinking-water supplies, it is particularly valuable to explain the occurrence of these contaminants in a human-health context.

In this report, measured concentrations of pesticides and VOCs are normalized to human-health benchmarks (MCL and HBSL values). It is common to present distributions of measured concentration data as in figures 4 and 5; however, the distributions of measured concentration data relative to human-health benchmarks have infrequently been presented as in figures 6-13. These types of figures allow for human-health related comparisons between compounds, well types, sampling regions, and land use. These types of figures can be created without HBSL values, instead using only USEPA drinking-water standards and guidelines as benchmarks. The addition of HBSL values, however, allows for the comparison of ground-water quality data in a human-health context for a larger suite of contaminants than those that have existing drinking-water standards and guidelines.

Additionally, HBSL values are scientifically defensible human-health benchmarks that provide a useful threshold for determining when measured contaminant concentrations in raw water approach or exceed concentrations that are relevant to human health. HBSL values can be used to assist with ground-water quality monitoring efforts and be used as planning tools to help (1) identify water resources with contaminant concentrations of potential human-health concern, (2) identify locations for future water-supply development, and (3) prioritize which contaminants detected at a site or in a study area are of potential human-health concern and may merit further study, monitoring, toxicity testing, regulation, or source control.

Summary

The primary objective of this report is to demonstrate the use of the Health-Based Screening Level (HBSL) approach as a tool for communicating water-quality data in a human-health context. A retrospective analysis of water-quality data was performed using ground-water quality data collected as part of the work conducted by the U.S. Geological Survey National Water-Quality Assessment (NAWQA) Program in the Long Island-New Jersey (LINJ) Coastal Drainages Study Unit. Another important objective of this report is to provide guidance on the use and interpretation of HBSL values and other human-health benchmarks in the analyses of water-quality data in other study areas. This guidance is intended primarily for USGS personnel conducting state- or local-scale water-quality studies; however, it can also be applied more generally by other agencies or organizations to facilitate the interpretation of water-quality data in a human-health context.

Ground-water samples were collected from 30 public-supply, 82 domestic, and 108 monitoring wells in New Jersey (3 wells in New York), and were analyzed for 97 pesticides and 85 volatile organic compounds (VOCs) during 1996-98. U.S. Environmental Protection Agency (USEPA) drinking-water standards or guidelines do not exist for 79 of these 182 compounds. Nonetheless, acceptable USEPA toxicity values are available for 39 of the 79 compounds; new HBSL values were calculated for these 39 unregulated compounds (that is, compounds without drinking-water standards) plus an additional 7 unregulated compounds for which updated toxicity data were available. Fourteen of these 46 compounds with new HBSL values were detected in the LINJ Study Unit. HBSL values were calculated using USEPA toxicity values and USEPA Office of Water methodologies. The use of HBSL values, in addition to USEPA standards and guidelines, increased the total number of pesticides and VOCs with human-health benchmarks analyzed in the study from 103 to 142 out of 182 compounds, a 21-percent increase.

Benchmark Quotient (BQ) values, defined as the ratio of the measured concentration of a detected contaminant to its Maximum Contaminant Level (MCL) value (for a regulated compound) or to its HBSL value (for an unregulated compound), were calculated for all detected pesticides and VOCs. Pesticides and VOCs were identified as being of potential human-health concern if their maximum detected concentrations in any well type were within a factor of 10 of their human-health benchmarks (that is, BQmax 0.1). Most (57 of 77) detected pesticides and VOCs with human-health benchmarks were detected at concentrations well below these levels (BQmax < 0.1), including 13 of the 14 detected compounds with new HBSL values. Twenty contaminants (6 pesticides and 14 VOCs) were identified as being of potential human-health concern in the study area because they had BQmax values greater than or equal to 0.1 for at least one well type. Four patterns of the occurrence of these 20 contaminants emerged.

1. Four contaminants—dieldrin, 1,2-dibromoethane, tetrachloroethylene, and trichloroethylene—were (1) measured in concentrations that met or exceeded human-health benchmarks and (2) frequently detected (that is, detected in more than 10 percent of samples) in raw (untreated) ground water that is used as drinking water (that is, public-supply wells and (or) domestic wells) and, therefore, are particularly relevant to human health.
2. Three contaminants—dinoseb, diuron, and 1,2-dibromo-3-chloropropane—were measured in concentrations that met or exceeded human-health benchmarks in monitoring and (or) domestic wells, but were not frequently detected in any well type.

3. Nine contaminants—atrazine, simazine, benzene, 1,1-dichloroethane, 1,1-dichloroethene, *cis*-1,2-dichloroethylene, 1,2-dichloropropane, methyl *tert*-butyl ether, and trichloromethane—were detected in measured concentrations that were less than, but within a factor of 10 of human-health benchmarks in at least one well type, and were frequently detected in public-supply or domestic wells.
4. Four contaminants—heptachlor epoxide, chloroethylene, 1,2-dichloroethane, and methylene chloride—were detected in measured concentrations that were less than, but within a factor of 10 of human-health benchmarks in monitoring or domestic wells, but were not frequently detected in any well type.

Eighteen of the 20 contaminants of potential human-health concern had Minimum Reporting Level (MRL) values less than their MCL or HBSL values for all well types, which permitted quantitation of these contaminants at concentrations that are relevant to human health. In contrast, 1,2-dibromo-3-chloropropane and 1,2-dibromoethane had MRL values greater than their MCL values in at least one well type, indicating the possibility that these two contaminants may be present, but not detected, in some samples at concentrations that are relevant to human health. In addition to the 20 contaminants of potential human-health concern identified in this study, deethylatrazine (a degradation product of the herbicides atrazine and propazine) is noteworthy because it was frequently detected in all well types, but it has no human-health benchmark for comparison with detected concentrations.

The detection frequencies of pesticides and VOCs generally were higher for public-supply well samples than for domestic-well samples. More contaminants were detected at concentrations within a factor of 10 of human-health benchmarks in samples from domestic wells (10 contaminants) than from public-supply wells (7 contaminants). Because water from domestic wells typically is consumed directly (that is, without treatment), this is an important finding and indicates that additional monitoring may be warranted for domestic wells.

Because multiple contaminants (53 to 75 pesticides plus VOCs) were detected in each type of well, initial efforts were undertaken to examine the occurrence of multiple contaminants in individual wells in relation to their respective human-health benchmarks. At least one pesticide or VOC with a human-health benchmark was detected in 208 of 220 (95 percent) individual wells. BQ values were calculated for detected compounds with human-health benchmarks in each well, and these values were used to determine the maximum BQ value (BQSiteMax) and the sum of all BQ values (BQSiteSum) for each individual well. In all wells, the median ratio of BQSiteMax to BQSiteSum values was approximately 1 for pesticides, and ranged from 0.77 for public-supply wells to 0.94 for domestic wells for VOCs, indicating that the BQSiteMax value makes up the majority of the sum. In other words, in this data set, the summed BQ value for all contaminants detected in a well was not substantially greater than the BQ value for the individual compound whose measured concentration in that well was highest relative to its human-health benchmark.

When the ground-water data were evaluated by individual well, BQSiteMax and BQSiteSum values were statistically greater (95-percent confidence level) for public-supply wells than for domestic and monitoring wells, likely because public-supply wells had the largest percentage of individual wells with pesticide or VOC concentrations that exceeded their human-health benchmarks. Although more contaminants were detected at concentrations with BQmax ≥ 0.1 in samples from domestic wells than from public-supply wells, BQSiteMax and BQSiteSum values were significantly lower (95-percent confidence level) for individual domestic wells than for individual public-supply and monitoring wells likely because (1) fewer domestic wells contained pesticides or VOCs detected at concentrations greater than human-health benchmarks than public-supply or monitoring wells, and (2) more domestic wells had no detections of compounds with human-health benchmarks than public-supply or monitoring wells.

The HBSL approach is an effective tool for placing water-quality data in a human-health context. As part of this pilot effort: (1) HBSL values increased the number of analyzed and detected compounds with human-health benchmarks; (2) guidance was provided on the use of HBSL values in the interpretation of water-quality data in a human-health context; (3) most detected contaminants were not identified as being of potential human-health concern, including 13 of the 14 contaminants with new HBSL values; and (4) contaminants of potential human-health concern that were identified were evaluated in the context of several factors, including the magnitude of BQ values, detection frequency, well type, and use of water.

Acknowledgments

The authors gratefully acknowledge the essential contributions of William G. Wilber, USGS NAWQA National Synthesis Coordinator, and John S. Zogorski, Chief of the USGS VOC National Synthesis Project, who spearheaded this pilot effort. The authors also acknowledge the collaboration and cooperation provided by individuals in several USEPA offices in the development of HBSL values, particularly Joyce Donohue from USEPA OW and Catherine Eiden from USEPA OPP, who were instrumental in HBSL development for compounds with multiple USEPA cancer classifications or toxicity values. Additionally, the authors thank Richard C. Hertzberg from USEPA ORD for his technical review of the "Health-Based Comparison of Wells with Multiple Contaminants" section. The authors are grateful to Mark Ayers, former LINJ Study-Unit Chief, for helping to develop collaborative relationships between USGS, NJDEP, and OHSU. The authors also acknowledge and thank Gregory C. Delzer, Michael J. Focazio, and Eric F. Vowinkel of USGS for their insightful technical reviews of this report. Finally, the authors thank Ruth M. Larkins who edited this report, and Ella Decker and Connie Ross who prepared this report for publication.

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Glossary

Benchmark Quotient (BQ) Ratio of the measured concentration of a detected contaminant to its Maximum Contaminant Level (MCL) value (for a regulated compound) or to its Health-Based Screening Level (HBSL) value (for an unregulated compound).

- **BQmax** Ratio of the maximum detected concentration of a contaminant in a given well type to its MCL or HBSL value.
- **BQmed-det** Ratio of the median of detected concentrations of a contaminant in a given well type to its MCL or HBSL value.
- **BQmed-all** Ratio of the median of all samples (including non-detections) of a contaminant in a given well type to its MCL or HBSL value.
- **BQSiteMax** Maximum of Benchmark Quotient values for detected contaminants in a given individual well.
- **BQSiteSum** Sum of all Benchmark Quotient values for detected contaminants in a given individual well.

Contaminants of Potential Human-Health Concern As used in this report, contaminants with maximum detected concentrations within a factor of 10 of applicable human-health benchmarks (that is, Maximum Benchmark Quotients (BQmax) greater than or equal to 0.1) for any well type.

Drinking-Water Guideline As used in this report, threshold concentrations that have no regulatory status, but are issued in an advisory capacity by the U.S. Environmental Protection Agency (USEPA) or state agencies.

Drinking-Water Standard As used in this report, threshold concentrations that are legally enforceable by the USEPA or state agencies.

Frequently Detected Compound As used in this report, a compound that is detected in at least 10 percent of samples from any given well type.

Health-Based Screening Level (HBSL) Estimates of benchmark concentrations (for noncarcinogens) or concentration ranges (for carcinogens) of contaminants in water that (1) may be of potential human-health concern; (2) can be used as threshold values against which measured concentrations of contaminants in ambient water samples can be compared; and (3) are consistent with USEPA Office of Water methodologies for setting drinking-water Lifetime Health Advisory and Risk-Specific Dose values (Toccalino and others, 2003; U.S. Environmental Protection Agency, 1988, 1993).

Human-Health Benchmarks As used in this report, a variety of drinking-water standards, guidelines, and threshold concentrations. These include USEPA and New Jersey Department of Environmental Protection (NJDEP) MCL values, USEPA Lifetime Health Advisory and Risk-Specific Dose values, NJDEP Ground Water Quality Criteria and Interim-Specific Ground Water Quality Criteria, and HBSL values developed collaboratively by the U.S. Geological Survey, USEPA, NJDEP, and Oregon Health & Science University.

Lifetime Health Advisory (Lifetime HA) The concentration of a chemical in drinking water that is not expected to cause any adverse noncarcinogenic effects over a lifetime of exposure (70 years). The Lifetime HA is based on exposure of a 70-kilogram adult consuming 2 liters of water per day, and assumes that only a portion (generally 20 percent) of the total exposure to a contaminant is from drinking water (U.S. Environmental Protection Agency, 1993 and 2004). A drinking-water guideline value issued by USEPA.

New HBSL As used in this report, HBSL values calculated for unregulated contaminants that (1) have no existing USEPA drinking-water guideline values or (2) have more recent USEPA toxicity data than that used to calculate existing USEPA drinking-water guideline values, resulting in different benchmark values.

Reference Dose (RfD) An estimate (with an uncertainty of perhaps one order of magnitude) of the daily exposure that is likely to be without appreciable risk of deleterious health effects in the human population (including sensitive subgroups) over an individual's lifetime (70 years) (U.S. Environmental Protection Agency, 1989b).

Regulated Compounds As used in this report, compounds with Federal and (or) state (specifically New Jersey) drinking-water standards.

Risk-Specific Dose (RSD) The drinking-water concentration associated with a specified cancer risk level (typically 1 in 10,000, 1 in 100,000, or 1 in 1,000,000), under certain exposure conditions: consumption of 2 liters per day of drinking water by a 70-kilogram body weight individual over a lifetime (70 years) (U.S. Environmental Protection Agency, 1993). A drinking-water guideline value issued by USEPA.

Slope Factor (SF) The cancer potency estimate for a compound as derived from the slope of the dose-response (carcinogenicity) data extrapolated to zero using an appropriate mathematical model (U.S. Environmental Protection Agency, 1989a,1993).

Unregulated Compounds As used in this report, compounds without Federal and (or) state (specifically New Jersey) drinking-water standards. Note that a compound that is unregulated in drinking water (federally, under the Safe Drinking Water Act) may be regulated in other contexts and under other statutes.

Appendixes

Appendix 1. U.S. Environmental Protection Agency and New Jersey MCL values (current as of August 2004) for regulated pesticides and VOCs analyzed in ground-water samples from the Long Island-New Jersey Study Unit.

[MCL, Maximum Contaminant Level; VOC, volatile organic compound; CASRN, Chemical Abstracts Service Registry Number; USEPA, U.S. Environmental Protection Agency; µg/L, micrograms per liter; NJ, New Jersey; LINJ, Long Island-New Jersey Study Unit]

Compound	CASRN	USEPA MCL[1] (µg/L)	NJ MCL[2] (µg/L)	Detected in LINJ
Pesticides				
Alachlor	15972-60-8	2	2	yes
Aldicarb	116-06-3	3	3	no
Aldicarb sulfone	1646-88-4	3	3	no
Aldicarb sulfoxide	1646-87-3	4	4	yes
Atrazine	1912-24-9	3	3	yes
Carbofuran	156-36-6	40	40	yes
Chlordane, technical	12789-03-6	2	.5	yes
2,4-dichlorophenoxyacetic acid (2,4-D)	94-75-7	70	70	yes
Dinoseb	88-85-7	7	7	yes
Endrin	72-20-8	2	2	no
Heptachlor	76-44-8	.4	.4	no
Heptachlor epoxide	1024-57-3	.2	.2	yes
Lindane	58-89-9	.2	.2	yes
Methoxychlor	72-43-5	40	40	no
Oxamyl	23135-22-0	200	200	no
Picloram	1918-02-1	500	500	yes
Simazine	122-34-9	4	4	yes
Toxaphene	8001-35-2	3	3	no
2-(2,4,5-trichlorophenoxy) propionic acid (2,4,5-TP)	93-72-1	50	50	yes
VOCs				
Benzene	71-43-2	5	1	yes
Bromodichloromethane	75-27-4	80	80	yes
Bromoform	75-25-2	80	80	yes
Chlorobenzene	108-90-7	100	50	yes
Chlorodibromomethane	124-48-1	80	80	yes
Chloroethylene	75-01-4	2	2	yes
1,2-Dibromo-3-chloropropane	96-12-8	.2	.2	yes
1,2-Dibromoethane	106-93-4	.05	.05	yes
1,2-Dichlorobenzene	95-50-1	600	600	yes
1,3-Dichlorobenzene	541-73-1	NAV	600	yes
1,4-Dichlorobenzene	106-46-7	75	75	yes

Appendix 1. U.S. Environmental Protection Agency and New Jersey MCL values (current as of August 2004) for regulated pesticides and VOCs analyzed in ground-water samples from the Long Island-New Jersey Study Unit. —Continued

[MCL, Maximum Contaminant Level; VOC, volatile organic compound; CASRN, Chemical Abstracts Service Registry Number; USEPA, U.S. Environmental Protection Agency; µg/L, micrograms per liter; NJ, New Jersey; LINJ, Long Island-New Jersey Study Unit]

Compound	CASRN	USEPA MCL[1] (µg/L)	NJ MCL[2] (µg/L)	Detected in LINJ
VOCs—Continued				
1,1-Dichloroethane	75-34-3	NAV	50	yes
1,2-Dichloroethane	107-06-2	5	2	yes
1,1-Dichloroethene	75-35-4	7	2	yes
cis-1,2-Dichloroethylene	156-59-2	70	70	yes
trans-1,2-Dichloroethylene	156-60-5	100	100	yes
1,2-Dichloropropane	78-87-5	5	5	yes
Ethylbenzene	100-41-4	700	700	yes
Methyl *tert*-butyl ether	1634-04-4	NAV	70	yes
Methylene chloride	75-09-2	5	3	yes
Naphthalene	91-20-3	NAV	300	yes
Styrene	100-42-5	100	100	yes
1,1,2,2-Tetrachloroethane	79-34-5	NAV	1	no
Tetrachloroethylene	127-18-4	5	1	yes
Tetrachloromethane	56-23-5	5	2	yes
Toluene	108-88-3	1,000	1,000	yes
1,2,4-Trichlorobenzene	120-82-1	70	9	no
1,1,1-Trichloroethane	71-55-6	200	30	yes
1,1,2-Trichloroethane	79-00-5	5	3	no
Trichloroethylene	79-01-6	5	1	yes
Trichloromethane	67-66-3	80	80	yes
Xylenes (sum of isomers)[3]	1330-20-7	10,000	1,000	yes

[1]U.S. Environmental Protection Agency, 2003a and 2004.

[2]New Jersey Department of Environmental Protection, 2000.

[3]Sum of Xylenes = *m*- & *p*-xylene (CASRN 108-38-3 & 106-42-3) + *o*-xylene (CASRN 95-47-6).

Appendix 2. HBSL values (current as of August 2004) for unregulated pesticides and VOCs analyzed in ground-water samples from the Long Island-New Jersey Study Unit.

[HBSL, Health-Based Screening Level; VOC, volatile organic compound; CASRN, Chemical Abstracts Service Registry Number; µg/L, micrograms per liter; LINJ, Long Island-New Jersey Study Unit; USEPA, U.S. Environmental Protection Agency; RSD, Risk-Specific Dose; OPP, Office of Pesticide Programs (USEPA); q1*, cancer potency factor; IRIS, Integrated Risk Information System; SF, oral slope factor; Lifetime HA, Lifetime Health Advisory; RfD, oral reference dose; HEAST, Health Effects Assessment Summary Tables (USEPA); OW, Office of Water (USEPA)]

Compound	CASRN	HBSL value or range[1] (µg/L)	Basis for HBSL (see Toccalino and others, 2003, for details on the HBSL approach)	New HBSL[2]	Detected in LINJ
			Pesticides		
Acetochlor	34256-82-1	2 to 200	RSD approach using OPP q1*	yes	yes
Acifluorfen[3]	50594-66-6	90	Lifetime HA approach using IRIS RfD	yes	no
Aldrin	309-00-2	0.002 to 0.2	RSD approach using IRIS SF	no	no
Azinphos-methyl	86-50-0	10	Lifetime HA approach using OPP RfD	yes	no
Benfluralin	1861-40-1	2,000	Lifetime HA approach using IRIS RfD	yes	yes
Bentazon	25057-89-0	200	Lifetime HA value	no	yes
Bromacil	314-40-9	90	Lifetime HA value	no	no
Bromoxynil	1689-84-5	10	Lifetime HA approach for Group C carcinogens using IRIS RfD	yes	no
Butylate	2008-41-5	400	Lifetime HA value	no	yes
Carbaryl[4]	63-25-2	40 to 4,000	RSD approach using OPP q1*	yes	yes
Chloramben	133904	100	Lifetime HA value	no	no
Chlorothalonil[5]	1897-45-6	5 to 500	RSD approach using OPP q1*	yes	no
Chlorpyrifos	2921-88-2	20	Lifetime HA value	no	no
Clopyralid	1702-17-6	4,000	Lifetime HA approach using OPP RfD	yes	no
Cyanazine	21725-46-2	1	Lifetime HA value	no	yes
Dacthal	1861-32-1	70	Lifetime HA value	no	yes
2,4-Dichlorophenoxybutyric acid (2,4-DB)	94-82-6	60	Lifetime HA approach using IRIS RfD	yes	no
p,*p*'-Dichlorodiphenyldichloroethane (*p*,*p*'-DDD)	72-54-8	0.1 to 10	RSD approach using IRIS SF	no	no
p,*p*'-Dichlorodiphenyldichloroethylene (*p*,*p*'-DDE)	72-55-9	0.1 to 10	RSD approach using IRIS SF	no	yes
p,*p*'-Dichlorodiphenyltrichloroethane (*p*,*p*'-DDT)	50-29-3	0.1 to 10	RSD approach using IRIS SF	no	no
Diazinon	333-41-5	.6	Lifetime HA value	no	no
Dicamba	1918-00-9	200	Lifetime HA value	no	yes
Dichlobenil	1194-65-6	9	Lifetime HA approach for Group C carcinogens using OPP RfD	yes	no
Dichlorprop	120-36-5	40	Lifetime HA approach using OPP RfD	yes	no
Dieldrin	60-57-1	0.002 to 0.2	RSD approach using IRIS SF	no	yes
Disulfoton	298-04-4	.3	Lifetime HA value	no	no
Diuron[6]	330-54-1	2 to 200	RSD approach using OPP q1*	yes	yes

Appendix 2. HBSL values (current as of August 2004) for unregulated pesticides and VOCs analyzed in ground-water samples from the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	HBSL value or range[1] (µg/L)	Basis for HBSL (see Toccalino and others, 2003, for details on the HBSL approach)	New HBSL[2]	Detected in LINJ
			Pesticides—Continued		
Endosulfan	115-29-7	40	Lifetime HA approach using IRIS RfD	yes	no
5-Ethyl dipropylthio-carbamate (EPTC)	759-94-4	200	Lifetime HA approach using IRIS RfD	yes	yes
Esfenvalerate	66230-04-4	100	Lifetime HA approach using OPP RfD	yes	no
Ethalfluralin	55283-68-6	30	Lifetime HA approach for Group C carcinogens using OPP RfD	yes	no
Ethoprophos	13194-48-4	1 to 100	RSD approach using OPP q1*	yes	no
Fluometuron	2164-17-2	90	Lifetime HA value	no	yes
Fonofos	944-22-9	10	Lifetime HA value	no	no
alpha-Hexachlorocyclo-hexane (alpha-HCH)	319-84-6	0.006 to 0.6	RSD approach using IRIS SF	no	no
Linuron	330-55-2	1	Lifetime HA approach for Group C carcinogens using IRIS RfD	yes	yes
Malathion	121-75-5	100	Lifetime HA value	no	no
2-Methyl-4-chlorophenoxy-acetic acid (MCPA)	94-74-6	4	Lifetime HA value	no	no
4-(2-Methyl-4-chlorophe-noxy) butyric acid (MCPB)	94-81-5	70	Lifetime HA approach using IRIS RfD	yes	no
Methiocarb	2032-65-7	40	Lifetime HA approach using OPP RfD	yes	no
Methomyl	16752-77-5	200	Lifetime HA value	no	yes
Metolachlor	51218-45-2	100	Lifetime HA value	no	yes
Metribuzin	21087-64-9	200	Lifetime HA value	no	yes
Mirex	2385-85-5	1	Lifetime HA approach using IRIS RfD	yes	no
Molinate	2212-67-1	1	Lifetime HA approach for Group C carcinogens using IRIS RfD	yes	no
Napropamide	15299-99-7	700	Lifetime HA approach using IRIS RfD	yes	yes
Norflurazon	27314-13-2	30	Lifetime HA approach for Group C carcinogens using IRIS RfD	yes	yes
Oryzalin	19044-88-3	40	Lifetime HA approach for Group C carcinogens using IRIS RfD	yes	no
Parathion	56-38-2	.02	Lifetime HA approach for Group C carcinogens using OPP RfD	yes	no
Parathion-methyl	298-00-0	2	Lifetime HA value	no	no
Pebulate	1114-71-2	50	Lifetime HA approach using OPP RfD	yes	no

Appendix 2. HBSL values (current as of August 2004) for unregulated pesticides and VOCs analyzed in ground-water samples from the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	HBSL value or range[1] (µg/L)	Basis for HBSL (see Toccalino and others, 2003, for details on the HBSL approach)	New HBSL[2]	Detected in LINJ
			Pesticides—Continued		
Pendimethalin	40487-42-1	30	Lifetime HA approach for Group C carcinogens using IRIS RfD	yes	yes
Phorate	298-02-2	4	Lifetime HA approach using OPP RfD	yes	no
Prometon	1610-18-0	100	Lifetime HA value	no	yes
Propachlor[7]	1918-16-7	1 to 100	RSD approach using OPP q1*	yes	no
Propanil	709-98-8	4	Lifetime HA approach for Group C carcinogens using IRIS RfD	yes	no
Propargite	2312-35-8	0.2 to 20	RSD approach using OPP q1*	yes	no
Propham	122-42-9	100	Lifetime HA value	no	no
Propoxur[8]	114-26-1	9 to 900	RSD approach using OPP q1*	yes	no
Propyzamide[9]	23950-58-5	2 to 200	RSD approach using OPP q1*	yes	no
2,4,5-Trichlorophenoxy-acetic acid (2,4,5-T)	93-76-5	70	Lifetime HA value	no	no
Tebuthiuron	34014-18-1	500	Lifetime HA value	no	yes
Terbacil	5902-51-2	90	Lifetime HA value	no	yes
Terbufos	13071-79-9	.9	Lifetime HA value	no	no
Thiobencarb	28249-77-6	70	Lifetime HA approach using IRIS RfD	yes	no
Triallate	2303-17-5	9	Lifetime HA approach for Group C carcinogens using IRIS RfD	yes	no
Triclopyr	55335-06-3	400	Lifetime HA approach using OPP RfD	yes	no
Trifluralin	1582-09-8	5	Lifetime HA value	no	yes
			VOCs		
Acetone	67-64-1	6,000	Lifetime HA approach using IRIS RfD	yes	yes
Acrylonitrile	107-13-1	0.06 to 6	RSD approach using IRIS SF	no	no
Bromochloromethane	74-97-5	90	Lifetime HA value	no	no
Bromomethane	74-83-9	10	Lifetime HA value	no	no
Carbon disulfide	75-15-0	700	Lifetime HA approach using IRIS RfD	yes	yes
1-Chloro-2-methylbenzene	95-49-8	100	Lifetime HA value	no	yes
4-Chlorotoluene	106-43-4	100	Lifetime HA value	no	no
Dichlorodifluoromethane	75-71-8	1,000	Lifetime HA value	no	yes
Ethyl ether	60-29-7	1,000	Lifetime HA approach using IRIS RfD	yes	yes
Ethyl methacrylate	97-63-2	600	Lifetime HA approach using HEAST RfD	yes	no

Appendix 2. HBSL values (current as of August 2004) for unregulated pesticides and VOCs analyzed in ground-water samples from the Long Island-New Jersey Study Unit.—Continued

Compound	CASRN	HBSL value or range[1] (µg/L)	Basis for HBSL (see Toccalino and others, 2003, for details on the HBSL approach)	New HBSL[2]	Detected in LINJ
VOCs—Continued					
Hexachlorobutadiene	87-68-3	1	Lifetime HA value	no	no
Hexachloroethane	67-72-1	1	Lifetime HA value	no	no
Isopropylbenzene	98-82-8	700	Lifetime HA approach using IRIS RfD	yes	yes
Methyl acrylate	96-33-3	200	Lifetime HA approach using HEAST RfD	yes	no
Methyl acrylonitrile	126-98-7	.7	Lifetime HA approach using IRIS RfD	yes	no
Methyl chloride	74-87-3	30	Lifetime HA value	no	yes
Methyl ethyl ketone	78-93-3	4,000	Lifetime HA value	no	yes
Methyl methacrylate	80-62-6	10,000	Lifetime HA approach using IRIS RfD	yes	no
1,1,1,2-Tetrachloroethane	630-20-6	70	Lifetime HA value	no	yes
1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	200,000	Lifetime HA approach using IRIS RfD	yes	yes
Trichlorofluoromethane	75-69-4	2,000	Lifetime HA value	no	yes
1,2,3-Trichloropropane	96-18-4	40	Lifetime HA value	no	yes

[1]HBSL range corresponds to a 10^{-6} to 10^{-4} cancer risk range for unregulated carcinogens.

[2]Unregulated compounds with new HBSLs do not currently (as of August 2004) have USEPA Lifetime HA or RSD values, except as noted. Unregulated compounds that do not have new HBSLs have previously published USEPA Lifetime HA values or USEPA RSD values from IRIS or OW.

[3]Based on sodium acifluorfen, CASRN 62476-59-9. Sodium acifluorfen has a USEPA OW 10^{-4} RSD value (100 µg/L). Sodium acifluorfen also has a new HBSL value (90 µg/L) based on an updated cancer classification published by USEPA OPP and toxicity data published by IRIS.

[4]Carbaryl has a USEPA Lifetime HA value (700 µg/L). Carbaryl also has a new HBSL range (40-4,000 µg/L) based on updated toxicity data published by USEPA OPP.

[5]Chlorothalonil has a USEPA OW 10^{-4} RSD value (150 µg/L). Chlorothalonil also has a new HBSL range (5-500 µg/L) based on updated toxicity data published by USEPA OPP.

[6]Diuron has a USEPA Lifetime HA (10 µg/L). Diuron also has a new HBSL range (2-200 µg/L) based on updated toxicity data published by USEPA OPP.

[7]Propachlor has a USEPA Lifetime HA (90 µg/L). Propachlor also has a new HBSL range (1-100 µg/L) based on updated toxicity data published by USEPA OPP.

[8]Propoxur has a USEPA Lifetime HA (3 µg/L). Propoxur also has a new HBSL range (9-900 µg/L) based on updated toxicity data published by USEPA OPP.

[9]Propyzamide has a USEPA Lifetime HA (50 µg/L). Propyzamide also has a new HBSL range (2-200 µg/L) based on updated toxicity data published by USEPA OPP.

Appendix 3. Unregulated pesticides and VOCs analyzed for in ground-water samples from the Long Island-New Jersey Study Unit that have no human-health benchmarks (as of August 2004).

[VOC, volatile organic compound; USEPA, U.S. Environmental Protection Agency; CASRN, Chemical Abstracts Service Registry Number; LINJ, Long Island-New Jersey Study Unit]

Compound	CASRN	Detected in LINJ
Pesticides		
Dacthal monoacid	887-54-7	no
Deethylatrazine	6190-65-4	yes
2,6-Diethylaniline	579-66-8	no
4,6-Dinitro-2-methylphenol	534-52-1	no
Fenuron	101-42-8	yes
3-Hydroxycarbofuran	16655-82-6	no
1-Naphthol	90-15-3	no
Neburon	555-37-3	no
cis-Permethrin	54774-45-7	no
Perthane	72-56-0	no
VOCs		
Bromobenzene	108-86-1	yes
Bromoethene	593-60-2	no
n-Butylbenzene	104-51-8	yes
sec-Butylbenzene	135-98-8	yes
tert-Butylbenzene	98-06-6	yes
Chloroethane	75-00-3	yes
3-Chloropropene	107-05-1	no
Dibromomethane	74-95-3	yes
trans-1,4-Dichloro-2-butene	110-57-6	no
1,3-Dichloropropane	142-28-9	yes
2,2-Dichloropropane	594-20-7	no
1,1-Dichloropropene	563-58-6	no
cis-1,3-Dichloropropene	10061-01-5	no
trans-1,3-Dichloropropene	10061-02-6	no
Diisopropylether	108-20-3	yes
Ethyl *tert*-butyl ether	637-92-3	no
1-Ethyl-2-methylbenzene	611-14-3	yes
2-Hexanone	591-78-6	no
Methyl iodide	74-88-4	yes
4-Methyl-2-pentanone	108-10-1	no
1-Methyl-4-isopropylbenzene	99-87-6	yes
tert-Pentyl methyl ether	994-05-8	yes
n-Propylbenzene	103-65-1	yes
Tetrahydrofuran	109-99-9	yes
1,2,3,4-Tetramethylbenzene	488-23-3	yes
1,2,3,5-Tetramethylbenzene	527-53-7	no
1,2,3-Trichlorobenzene	87-61-6	no
1,2,3-Trimethylbenzene	526-73-8	yes
1,2,4-Trimethylbenzene	95-63-6	yes
1,3,5-Trimethylbenzene	108-67-8	yes

Prepared for the National Water-Quality Assessment Program, by the Oregon Health & Science University

Text layout by Ella M. Decker.

Graphics by Connie J. Ross.

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