HISTORICAL RECONSTRUCTION OF PCE-CONTAMINATED DRINKING WATER USING PROBABILSITIC ANALYSIS AT U.S. MARINE CORPS BASE CAMP LEJEUNE, NORTH CAROLINA*

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ABSTRACT

The historical reconstruction process is used to derive contaminant concentrations and exposure levels needed as input by health scientists conducting retrospective epidemiological studies—models are an integral part of this process. However, the models and associated calibrated parameters are inherently uncertain because they are based on limited historical data and information. This gives rise to the question, what is the reliability of the historically reconstructed estimates of contaminant concentrations determined using calibrated models? To answer this question and address the overarching issues of model and parameter variability and uncertainty, a probabilistic analysis is used to generate uncertainties of model inputs (e.g., hydraulic conductivity or contaminant source mass loading rate) so that estimates of uncertainties in model outputs (e.g., water level or contaminant concentrations in groundwater) can be made. In this paper, the authors describe the application of a probabilistic analysis using Monte Carlo simulations to assess model uncertainty and parameter variability. The probabilistic analysis is applied to groundwater-flow and contaminant fate and transport models (MODLFOW and MT3DMS, respectively) as

* The findings and conclusions in this paper are those of the authors and do not necessarily represent the views of the Agency for Toxic Substances and Disease Registry.

part of an ongoing health study—exposure to volatile organic compounds in drinking water and specific birth defects and childhood cancers—being conducted by the Agency for Toxic Substances and Disease Registry at U.S. Marine Corps Base Camp Lejeune, North Carolina (Figure 1). Results of probabilistic analysis are presented in terms of the probability of occurrence tetrachloroethylene (PCE) contamination in groundwater, the probability of exceeding the current maximum contaminant level for PCE in finished drinking water (5 micrograms per liter), and the range of expected PCE concentrations in finished drinking water during the historical period of interest (1968–1985) for the health study.

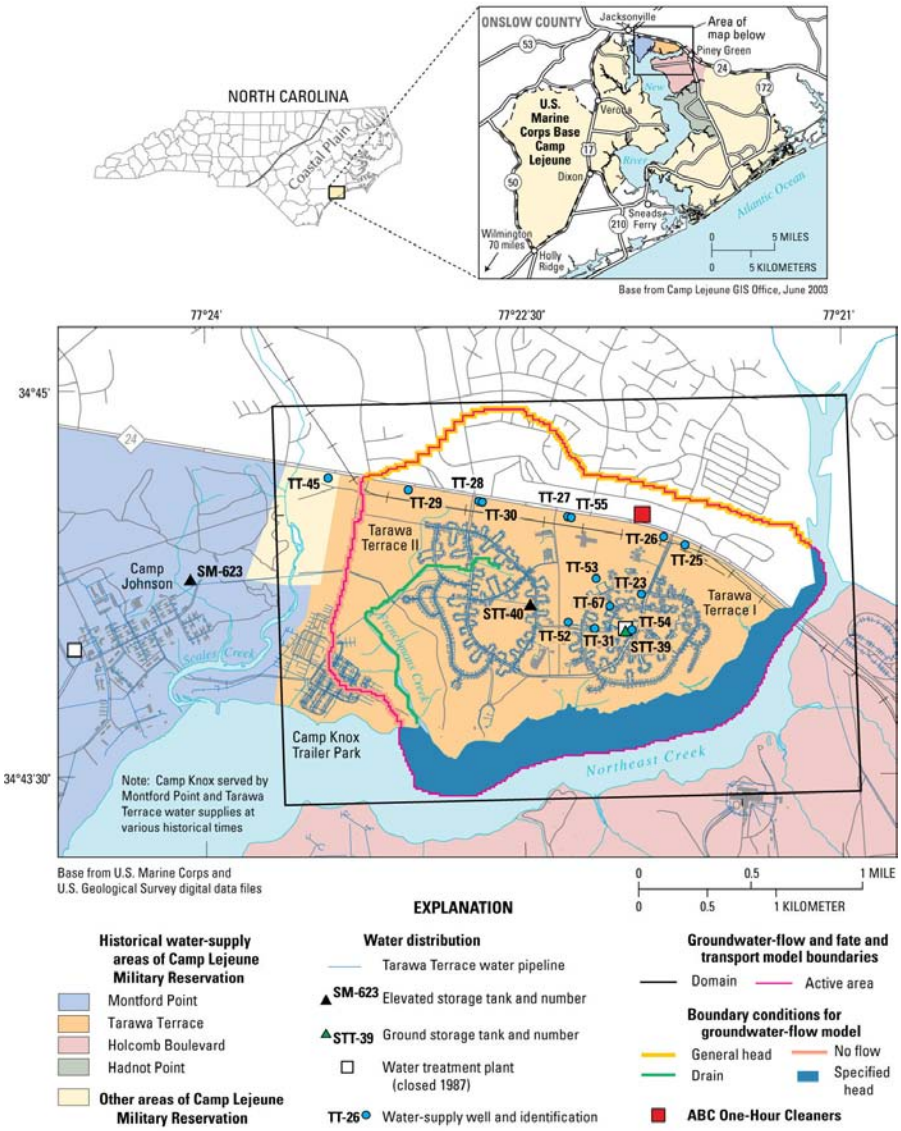

Figure 1. Water-supply areas, groundwater-flow modeling area, and water-supply facilities used for historical reconstruction analyses (from Maslia et al. 2007).

INTRODUCTION AND HISTORICAL BACKGROUND

Three water-distribution systems have historically supplied drinking water to family housing at U.S. Marine Corps Base Camp Lejeune, North Carolina. Two of the systems were contaminated with volatile organic compounds (VOCs). Tarawa Terrace was contaminated mostly with tetrachloroethylene (PCE), and Hadnot Point was contaminated mostly with trichloroethylene (TCE). The analyses and results presented in this paper refer solely to Tarawa Terrace and vicinity. Historical information and data have indicated that one source of contamination—ABC One-Hour Cleaners (Figure 1)—was responsible for contaminating Tarawa Terrace water-supply wells (Shiver 1985). Water-supply data and operational information indicate that Tarawa Terrace wells supplied water solely to the Tarawa Terrace water treatment plant (WTP). Additionally, the Tarawa Terrace water-distribution system was operated independently of the other two water-distribution systems.

Because scientific data relating to the harmful effects of VOCs on a child or fetus are limited, the Agency for Toxic Substances and Disease Registry (ATSDR), an agency of the U.S. Department of Health and Human Services, is conducting an epidemiological study to evaluate potential associations between in utero and infant (up to 1 year of age) exposures to VOCs in contaminated drinking water at Camp Lejeune and specific birth defects and childhood cancers. The study includes births occurring during the period 1968–1985 to women who were pregnant while they resided in family housing at Camp Lejeune. Owing to limited measurements of contaminant and exposure data to support the epidemiological study, ATSDR is using modeling techniques to reconstruct historical conditions of groundwater flow, contaminant fate and transport, and the distribution of drinking water contaminated with VOCs delivered to family housing areas. Using water-modeling techniques in such a process is referred to as historical reconstruction (Maslia et al. 2001).

APPROACH FOR RECONSTRUCTING HISTORICAL CONCENTRATIONS

A simulation or modeling approach was used to reconstruct and estimate (quantify) historical concentrations of PCE in finished water that was delivered to residents of Tarawa Terrace. For this study, the concentration of treated water at the WTP is considered the same as the concentration of water delivered to a person's home. In using a simulation approach the following models were applied to the study area and calibrated:

- MODFLOW-96 (Harbaugh and McDonald 1996): simulation of steady-state and transient groundwater flow, and
- MT3DMS (Zheng and Wang 1999): simulation of PCE as a single-specie contaminant dissolved in groundwater.

Historically, groundwater from all water-supply wells was mixed and treated at the Tarawa Terrace WTP. Therefore, a materials mass balance approach, using principles of continuity and conservation of mass (Masters 1998), was used to compute the concentration of PCE in finished drinking water delivered to residents of Tarawa Terrace. A flowchart of the historical reconstruction process used to compute PCE concentrations in finished water at the Tarawa Terrace WTP is shown in Figure 2.

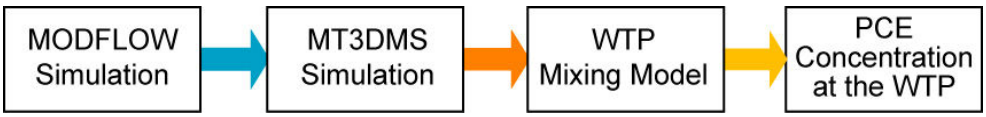

Figure 2. Flowchart of the historical reconstruction process used to compute tetrachloroethylene (PCE) concentrations in finished water at the Tarawa Terrace water treatment plant (WTP).

Calibration of the models used for the Tarawa Terrace analyses was accomplished in a hierarchical or step-wise approach consisting of four successive stages or levels. Simulation results achieved for each calibration level were refined by adjusting model parameter values and comparing these results with simulation results of previous levels until results at all levels were within ranges of preselected calibration targets or measures. The step-wise order of model-calibration levels consisted of simulating (1) predevelopment (steady or nonpumping) groundwater-flow conditions, (2) transient (time varying or pumping) groundwater-flow conditions, (3) the fate and transport (migration) of PCE from its source at ABC One-Hour Cleaners to water-supply wells, and (4) the concentration of PCE in finished water at the Tarawa Terrace WTP—water from the Tarawa Terrace WTP that was delivered to residents living in family housing. Details describing and summarizing the development and calibration of the aforementioned models are provided in the following references: Faye (2008), Faye and Valenzuela (2007), and Maslia et al. (2007).

RESULTS OF WATER-MODELING ANALYSES

A graph showing simulated concentrations of PCE at Tarawa Terrace water-supply wells from the beginning of operations at ABC One-Hour Cleaners through the closure of the wells and the WTP is shown in Figure 3. Simulated PCE concentrations in water-supply well TT-26 exceeded the current maximum contaminant level (MCL) for PCE of 5 µg/L during January 1957 (simulated value is 5.2 µg/L) and reached a maximum simulated value of 851 µg/L during July 1984. The mean simulated PCE concentration in water-supply well TT-26 for its entire period of operation was 351 µg/L. The mean simulated PCE concentration for the period exceeding the current MCL of 5 µg/L—January 1957 to January 1985—was 414 µg/L. This represents a duration of 333 months (27.7 years). These results are summarized in Table 1 along with simulated results for water-supply wells TT-23 and TT-25. It should be noted that although simulation results indicate several water-supply wells were contaminated with PCE (wells TT-23, TT-25, TT-31, TT-54, and TT-67), by far, the highest concentration of PCE and the longest duration of contamination occurred in water-supply well TT-26 (Figure 3).

Table 1. Summary statistics for tetrachloroethylene (PCE) contamination of selected Tarawa Terrace water-supply wells and water treatment plant (WTP) based on calibrated model simulation (from Maslia et al. 2007).

[MCL, maximum contaminant level; µg/L, micrograms per liter]

Water supply	Month, year, and duration exceeding MCL[1]	Month and year of maximum value and maximum concentration, in µg/L	Average concentration, in µg/L[2]
TT-23	Aug. 1984–Apr. 1985 8 months[3]	Apr. 1985 274	252
TT-25	Jul. 1984–Feb. 1987 32 months	Feb. 1987 69	33
TT-26	Jan. 1957–Jan. 1985 333 months[4]	Jul. 1984 851	414
WTP	Nov. 1957–Feb.1987 346 months	Mar.1984 183	70

[1]Current MCL for PCE is 5 µg/L, effective date July 6, 1992 (40 CFR, Section 141.60, Effective Dates, July 1, 2002, ed.)
[2]For periods exceeding 5 µg/L when water-supply well was operating.
[3]Water-supply well TT-23 was not operating in February 1985.
[4]Water-supply well TT-26 was not operating July–August 1980 and January–February 1983.

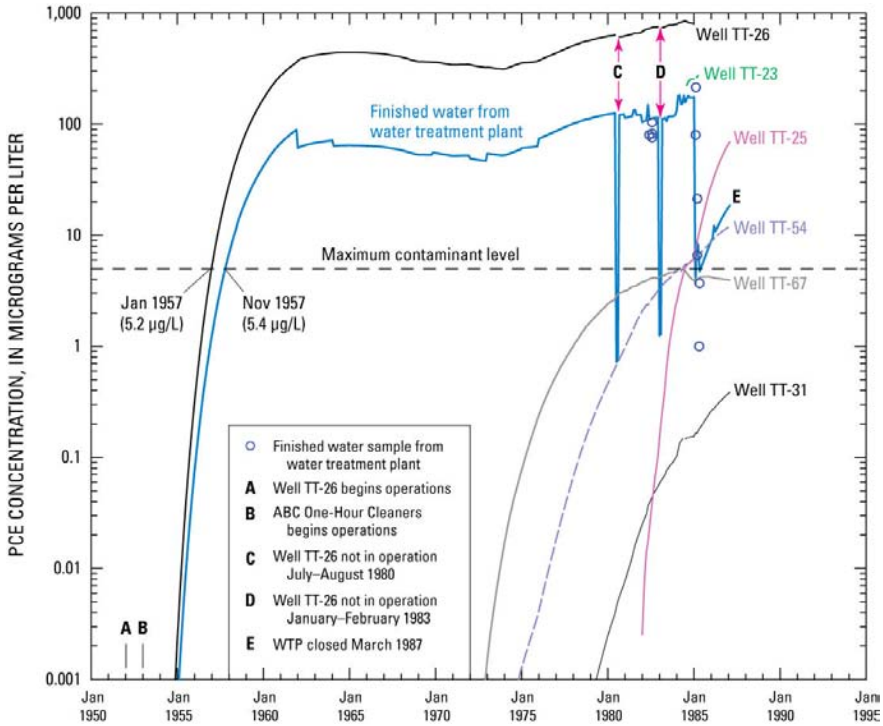

Figure 3. Simulated and measured concentration of tetrachloroethylene (PCE) at Tarawa Terrace water-supply wells and the water treatment plant (from Maslia et al. 2007).

CONFIDENCE IN SIMULATION RESULTS

The models and model results described above are based on limited field data and literature-derived values. Therefore, the models and results are characterized by uncertainty (lack of knowledge about specific factors) and variability (observed differences that can be attributed to differences in model parameters). Under such circumstances, good modeling practice requires that evaluations be conducted to ascertain the confidence in models by assessing uncertainties associated with the modeling process and with the outcomes attributed to models (Saltelli et al. 2000). With respect to model simulations at Tarawa Terrace, the availability of data to thoroughly characterize and describe model parameters and operations of water-supply wells was considerably limited. This gives rise to the question, what confidence does one have in the historically reconstructed estimates of concentration such as results shown in Figure 3? To answer this question and address issues of uncertainty and variability, exhaustive sets of additional simulations were conducted to estimate (quantify) confidence in models and their results. One approach used to conduct these additional simulations and estimate confidence in model results was a probabilistic analysis.

For the probabilistic analysis, Monte Carlo and sequential Gaussian simulation were applied to calibrated model parameters derived for the groundwater flow (Faye and Valenzuela 2007) and fate and transport models (Faye 2008). Two probabilistic analysis scenarios were conducted. For Scenario 1, groundwater pumpage uncertainty was *excluded* from the analysis, while eight other parameters were assumed to be uncertain and variable: (1) horizontal hydraulic conductivity, (2) recharge rate, (3) effective porosity, (4) bulk density, (5) distribution coefficient, (6) dispersivity, (7) reaction rate, and (8) PCE mass-loading rate. For Scenario 2, groundwater pumpage uncertainty (Figure 4) was *included* in the analysis in addition to the eight aforementioned parameter variants. The rationale for assuming that pumpage is a variant is based on pumping schedule variation analyses conducted by Wang and Aral (2007) indicating that such variations could cause significant change in the concentration of PCE at the WTP. Comparison of Scenario 1 and Scenario 2 pumpage schemes is shown in Figure 4. The variation of pumpage for the Scenario 2 graph is an example of a Monte Carlo generation of monthly pumpage that is based on a statistical analysis of recorded monthly pumpage for the years 1978, 1980, 1981, 1983, and 1984. Statistical descriptions of input parameter distributions and details describing the programmatic sequences using the MODFLOW (Harbaugh and McDonald 1996; Harbaugh et al. 2000) and MT3DMS (Zheng and Wang 1999) models and Monte Carlo simulation to conduct probabilistic analyses are provided in Maslia et al. (2007) and Maslia et al. (2008 In Press).

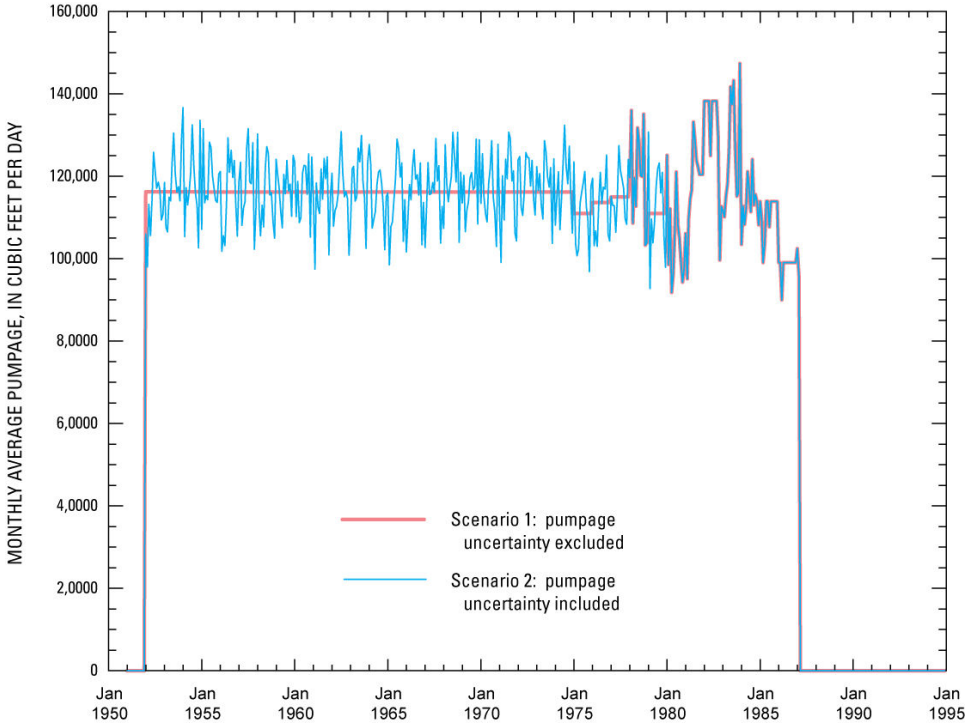

Figure 4. Comparison of pumpage scenarios: Scenario 1, pumpage uncertainty excluded and Scenario 2, pumpage uncertainty included (from Maslia et al. 2008 In Press).

Scenario 1: Pumpage Uncertainty Excluded

For Scenario 1, 840 realizations were conducted as part of the probabilistic analysis simulations; 510 realizations yielded plausible solutions—about a 61% success rate. A solution was determined to be not plausible or not successful if, for example, a water-supply well dried up during any part of the simulation. An example of probabilistic results derived by using Monte Carlo analysis for Scenario 1 (pumpage uncertainty excluded) is shown in Figure 5. In this illustration, the concentration of PCE in finished water is shown as a range of most likely values for each month that the Tarawa Terrace WTP was in operation—January 1953–February 1987. As can be seen, the probabilistic results form a very narrow range or band around simulated concentration values obtained from running the groundwater-flow and fate and transport models without considering uncertainty and variability. The range of PCE concentrations in finished water for each month of WTP operations represents 95 percent of Monte Carlo simulations (yellow band in Figure 5). That is, there is a 95 percent probability that PCE concentrations in finished water delivered to residents of Tarawa Terrace from the WTP were within the band or range of values shown in Figure 5 for each month that the WTP was operating.

Two specific results shown in Figure 5 are worthy of further explanation. First, PCE concentrations in WTP finished water most likely exceeded the MCL for PCE of 5 µg/L for the first time during October 1957–August 1958 (95 percent probability). This range includes the date of November 1957 derived without considering

uncertainty and variability. Second, the PCE concentration in WTP finished water during January 1985, simulated using the probabilistic analysis, ranges from 110–251 µg/L (95 percent of Monte Carlo simulations). This range includes the calibrated value of 176 µg/L (derived without considering uncertainty and variability) and the maximum measured value of 215 µg/L. Therefore, these probabilistic analysis results—obtained by using Monte Carlo simulation—provide a sense of confidence in the historically reconstructed PCE concentrations that were delivered to residents of Tarawa Terrace in finished water from the WTP.

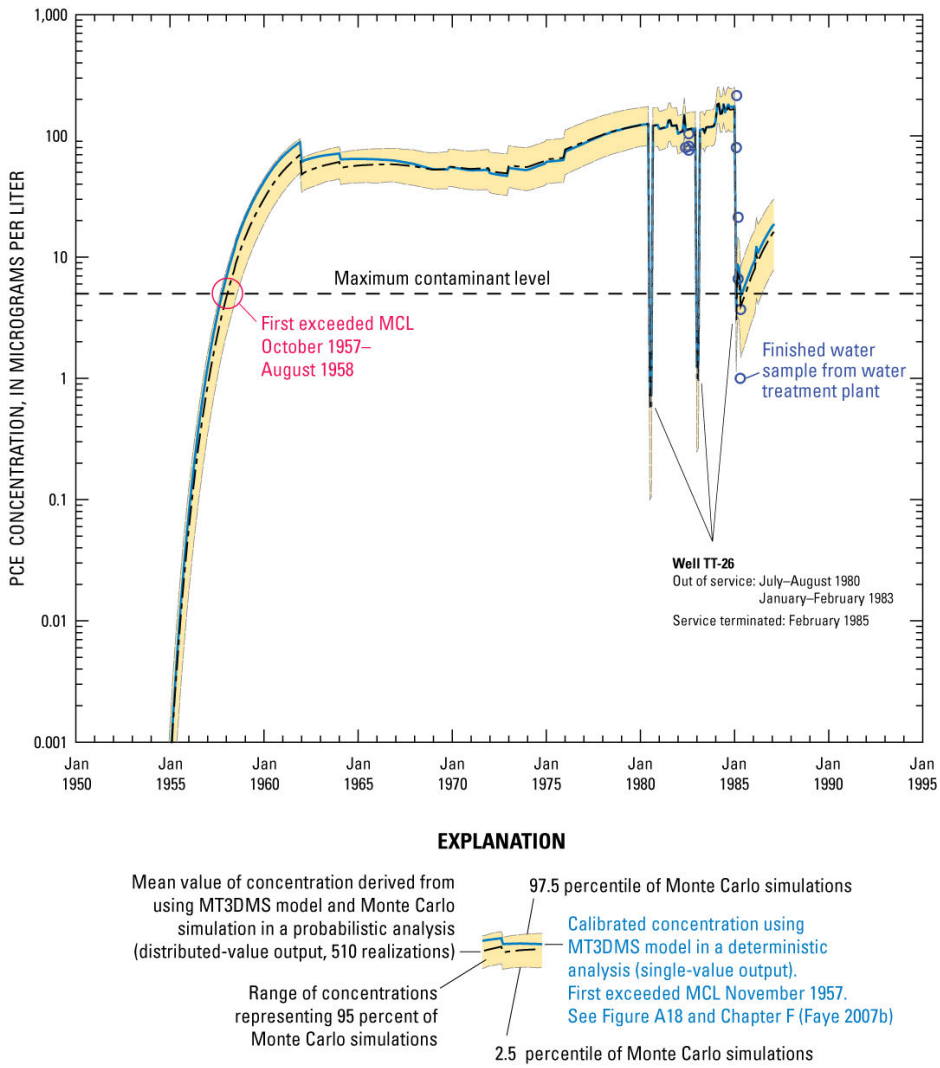

Figure 5. Concentrations of tetrachloroethylene (PCE) in finished water at the Tarawa Terrace water treatment plant derived from probabilistic analysis using Monte Carlo simulation: Scenario 1, pumpage uncertainty excluded (from Maslia et al. 2007).

Scenario 2: Pumpage Uncertainty Included

For scenario 2, 700 realizations were conducted as part of the probabilistic analysis simulations; 684 realizations yielded plausible solutions—about a 95% success rate.

For Scenario 2, 95% of the Monte Carlo simulations indicated that the simulated concentration of PCE in finished water at the WTP first exceeded the current MCL of 5 mg/L during November 1957–December 1958. The mean PCE MCL exceedance date for Scenario 2 is April 1958. This is five months later than results obtained from the calibrated model (Faye and Valenzuela 2007) and two months later than Scenario 1 simulations (Maslia et al. 2007) where pumpage uncertainty was not included. Comparison of concentrations of PCE in finished water at the Tarawa Terrace WTP derived from probabilistic analysis using Monte Carlo simulation for the calibrated model, Scenario 1, and Scenario 2 pumpage conditions are shown in Figure 6.

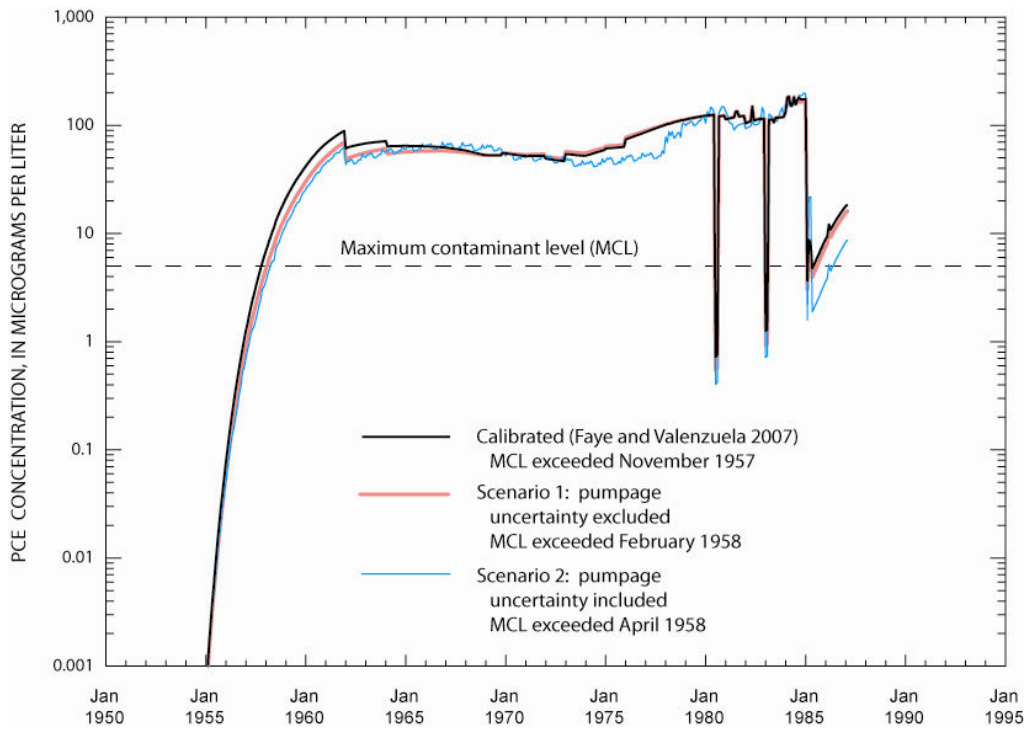

Figure 6. Concentrations of tetrachloroethylene (PCE) in finished water at the Tarawa Terrace water treatment plant derived from probabilistic analysis using Monte Carlo simulation for calibrated model, Scenario 1, and Scenario 2 pumpage conditions (from Wang and Aral 2007; Maslia et al. 2008 In Press).

For purposes of a health study or exposure assessment, epidemiologists and health scientists are interested in obtaining information on the probability that a person or population was exposed to a contaminant exceeding a given health guideline or criteria. For example, the probability that residents of Tarawa Terrace were exposed to drinking water contaminated with PCE exceeding an MCL of 5 μg/L. To address this issue, Monte Carlo simulation results described above can be analyzed in terms of a complementary cumulative probability function. This analysis yields a series of probability "type curves" (Figure 7). The complementary cumulative probability function describes the probability of exceeding a certain value or answers the question: how often is a random variable (e.g., the concentration of PCE in finished water) above a certain value? Using results shown in Figure 7, the probability that the

PCE concentration in finished water at the Tarawa Terrace WTP exceeded a value of 5 μg/L during January 1958 is determined in the following manner: (1) locate the probabilistic type curves for January 1958 in Figure 7, (2) locate the 5 μg/L PCE concentration along the x-axis of the graph, (3) follow the vertical line until it intersects with the January 1958 complementary cumulative probability function type curve for either the Scenario 1 or Scenario 2 simulation, and (4) follow the horizontal line until it intersects the y-axis. In this study, Scenario 1 results (pumpage uncertainty excluded) indicate a 38% probability of exceeding the MCL for PCE during January 1958 and Scenario 2 results (pumpage uncertainty included) indicate an 11% probability of exceeding the MCL for PCE during January 1958. Thus, the difference in the probability of exceedance is caused by the variation of pumping schedules that is accounted for in the Scenario 2 simulations because pumping is treated as a variant for the probabilistic analysis.

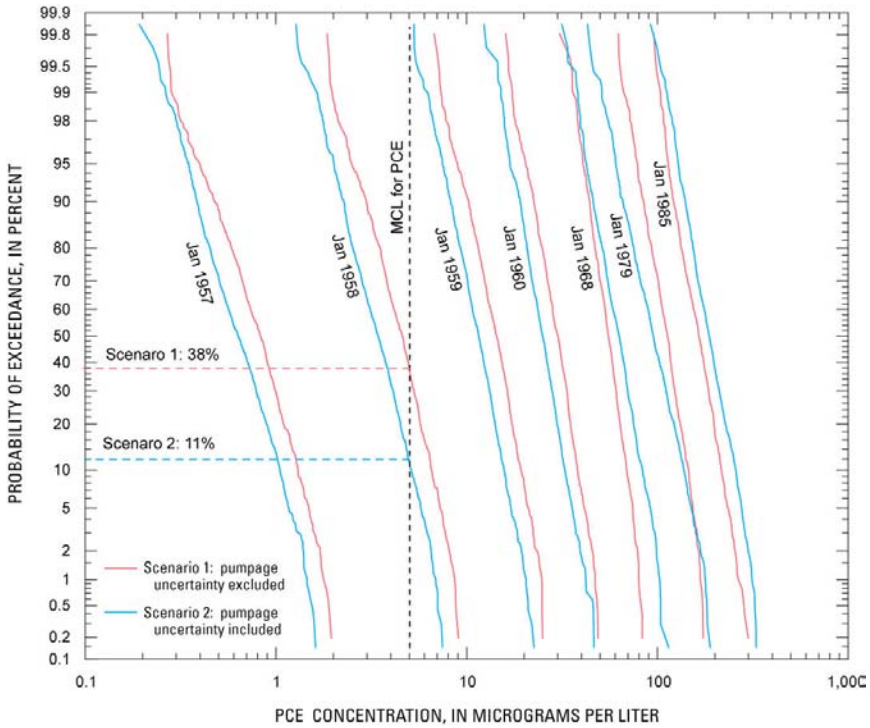

Figure 7. Probability of exceeding concentrations of tetrachloroethylene (PCE) in finished water at the Tarawa Terrace water treatment plant derived from probabilistic analysis using Monte Carlo simulation for Scenario 1 and Scenario 2 pumpage conditions (from Wang and Aral 2007; Maslia et al. 2008 In Press).

SUMMARY AND CONCLUSIONS

Results of a historical reconstruction analysis have been presented for the Tarawa Terrace area of U.S. Marine Corps Base Camp Lejeune, North Carolina. The analyses were conducted to support an epidemiological study being conducted by the Agency for Toxic Substances and Disease Registry (ATSDR) to evaluate potential associations between in utero and infant (up to 1 year of age) exposures to volatile

organic compounds in contaminated drinking water at Camp Lejeune and specific birth defects and childhood cancers. To support the study, groundwater fate and transport models were developed and calibrated to reconstruct the migration of tetrachloroethylene (PCE) from its source at ABC One-Hour Cleaners to Tarawa Terrace water-supply wells (Figure 1). A mixing model was used to compute the flow-weighted concentration of PCE in finished water at the water treatment plant (WTP) that was distributed to residents of Tarawa Terrace housing (Figure 2). As part of the historical reconstruction process, a series of probabilistic analyses, using Monte Carlo simulation, were conducted to assess parameter and model uncertainty. Through the analysis and comparison of results from different probabilistic analyses, including assessing the impact of water-supply well pumping schedule uncertainty, the following conclusions can be made: (1) the PCE concentration obtained from the calibrated models is reasonable, (2) the most likely time for PCE concentration in the Tarawa Terrace WTP to exceed the current maximum contaminant level (5 μg/L) ranges from the end of 1957 through the beginning of 1958, and (3) pumping schedule variation and uncertainty can cause significant changes to the PCE concentration at the WTP.

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