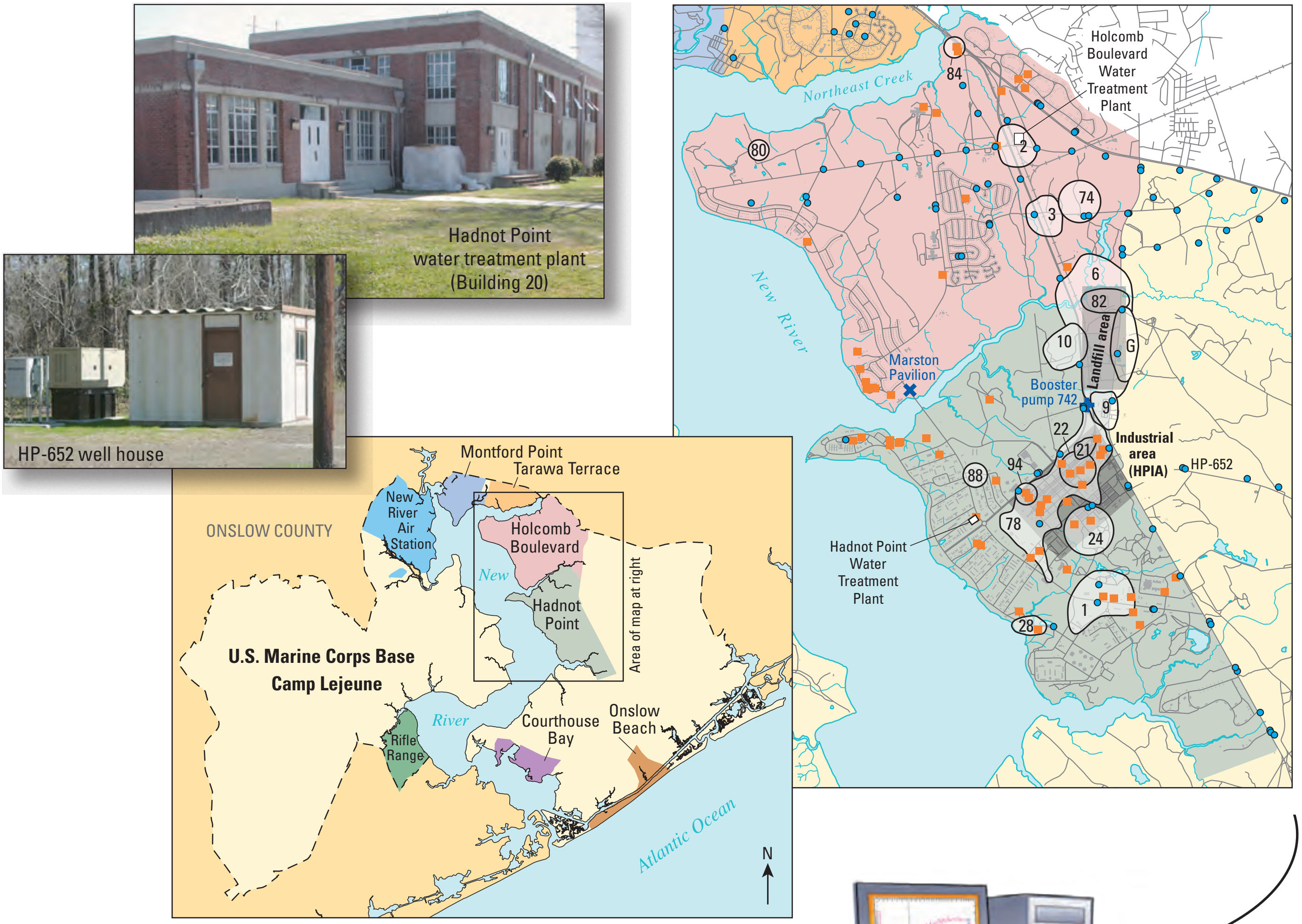
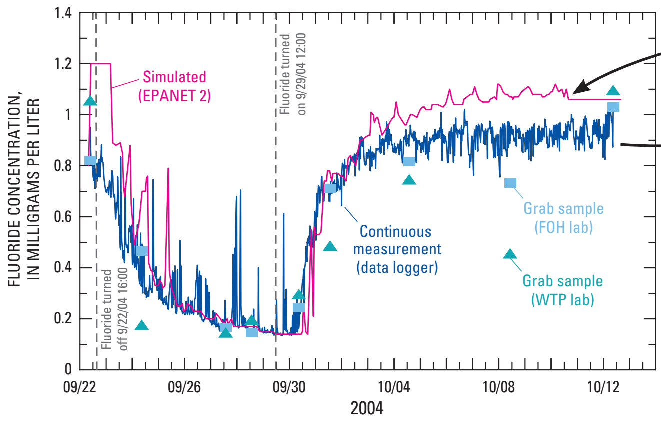
Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina

Chapter A–Supplement 5

Theory, Development, and Application of Linear Control Model Methodology to Reconstruct Historical Contaminant Concentrations at Selected Water-Supply Wells





ATSDR
AGENCY FOR TOXIC SUBSTANCES AND DISEASE REGISTRY

Atlanta, Georgia–March 2013

Front cover: Historical reconstruction process using data, information sources, and water-modeling techniques to estimate historical contaminant concentrations.

Maps: U.S. Marine Corps Base Camp Lejeune, North Carolina; Holcomb Boulevard and Hadnot Point areas showing extent of sampling at Installation Restoration Program sites (white numbered areas), above-ground and underground storage tank sites (orange squares), and water-supply wells (blue circles).

Photograph (upper): Hadnot Point water treatment plant (Building 20).

Photograph (lower): Well house building for water-supply well HP-652.

Graph: Measured fluoride data and simulation results for Paradise Point elevated storage tank (S-2323) for tracer test of the Holcomb Boulevard water-distribution system, September 22–October 12, 2004; simulation results obtained using EPANET 2 water-distribution system model assuming last-in first-out plug flow (LIFO) storage tank mixing model. [WTP lab, water treatment plant water-quality laboratory; FOH lab, Federal Occupational Health Laboratory]

Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina

Chapter A–Supplement 5

Theory, Development, and Application of Linear Control Model Methodology to Reconstruct Historical Contaminant Concentrations at Selected Water-Supply Wells

By Jiabao Guan, Barbara A. Anderson, Mustafa M. Aral, and Morris L. Maslia

Agency for Toxic Substances and Disease Registry
U.S. Department of Health and Human Services
Atlanta, Georgia

March 2013

AGENCY FOR TOXIC SUBSTANCES
AND DISEASE REGISTRY

Authors

Jiabao Guan, PhD, PE
Senior Research Engineer
Georgia Institute of Technology
School of Civil and Environmental Engineering
Multimedia Environmental Simulations Laboratory
Atlanta, Georgia

Barbara A. Anderson, MSEnvE, PE
Environmental Health Scientist
Agency for Toxic Substances and Disease Registry
Division of Community Health Investigations
Atlanta, Georgia

Mustafa M. Aral, PhD, PE, Phy
Director and Professor
Georgia Institute of Technology
School of Civil and Environmental Engineering
Multimedia Environmental Simulations Laboratory
Atlanta, Georgia

Morris L. Maslia, MSCE, PE, D.WRE, DEE
Research Environmental Engineer and Project Officer
Agency for Toxic Substances and Disease Registry
Division of Community Health Investigations
Exposure-Dose Reconstruction Project
Atlanta, Georgia

For additional information write to:

Project Officer
Exposure-Dose Reconstruction Project
Division of Health Assessment and Consultation (proposed)
Agency for Toxic Substances and Disease Registry
4770 Buford Highway, Mail Stop F-59
Atlanta, Georgia 30341-3717

Suggested citation

Guan J, Anderson BA, Aral MM, and Maslia ML. Theory, Development, and Application of Linear Control Model Methodology to Reconstruct Historical Contaminant Concentrations at Selected Water-Supply Wells—Supplement 5. In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

Contents

Figures

Tables (Table S5.3 is in back of report)

See the Glossary section in Chapter A of this report for definitions of terms and abbreviations used throughout this supplement.

Use of trade names and commercial sources is for identification only and does not imply endorsement by the Agency for Toxic Substances and Disease Registry, the U.S. Department of Health and Human Services, or the U.S. Geological Survey.

Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina

Chapter A–Supplement 5

Theory, Development, and Application of Linear Control Model Methodology to Reconstruct Historical Contaminant Concentrations at Selected Water-Supply Wells

By Jiabao Guan,[1] Barbara A. Anderson,[2] Mustafa M. Aral,[1] and Morris L. Maslia[2]

Introduction

In a review of the Agency for Toxic Substances and Disease Registry (ATSDR) water-modeling analyses for the Tarawa Terrace study area of U.S. Marine Corps Base (USMCB) Camp Lejeune, North Carolina, the National Research Council (2009) suggested that ATSDR explore methods of analyses for groundwater flow and contaminant fate and transport modeling that were simpler than the traditional numerical methods. A screening-level method that uses linear control model methodology was developed in response to this suggestion.

This report provides the mathematical development of a linear state-space representation of a contaminated aquifer system, designated in this report as a linear control model (LCM). The utility and accuracy of this novel approach are verified using synthetic data from a detailed numerical groundwater model previously developed for the Tarawa Terrace study (Maslia et al. 2007, Jang and Aral 2008), and subsequently applied to reconstruct the history of chlorinated solvent contamination at a key water-supply well, designated HP-651, in the Hadnot Point landfill (HPLF) area at USMCB Camp Lejeune. Water-supply well HP-651 was shut down in early 1985 when chlorinated solvents were detected in the well. The LCM approach uses the historical operating schedule of HP-651 in conjunction with measured contaminant concentrations in groundwater during 1985–2004 to reconstruct the history of contaminants in the well prior to 1985.

Reconstructing the historical concentration of contaminants in a groundwater system is a challenging problem, particularly when historical contaminant data and contaminant source information are limited. By proposing a linear discrete system state equation to approximately describe the aquifer system, the historical reconstruction problem is transformed into a system identification problem that can be solved by using control theory principles. The LCM approach described herein requires very little initial parameter definition and calibration. Using the LCM approach, a reasonable estimate of historical contaminant concentrations in groundwater can be obtained fairly early in a project, before significant investments are made to characterize model and aquifer parameters, define the hydrogeologic framework for multilayer aquifers, select boundary conditions, and calibrate the groundwater flow and contaminant transport models. Such investments, which are hallmarks of traditional numerical modeling of complex groundwater systems, are typically time-consuming and costly.

The LCM approach provides a screening level model that is localized in a specific hydrogeologic area of interest. It is a useful tool to (1) improve understanding of the system, which is one of the most important aspects of any model, (2) contribute timely information to the decision process of whether to conduct more detailed modeling, and (3) provide a point of comparison for other modeling approaches that are applied to the system.

---

[1] Georgia Institute of Technology, School of Civil and Environmental Engineering, Atlanta, Georgia.

[2] Agency for Toxic Substances and Disease Registry, Atlanta, Georgia.

Background

As outlined in Maslia et al. (2013), ATSDR is conducting epidemiological studies to evaluate the potential for health effects from exposures to volatile organic compounds (VOCs) in finished water[3] supplied to family housing units at USMCB Camp Lejeune. The core study period for the epidemiological studies is 1968–1985. Because exposure data—measured contaminant concentrations in the finished water—are limited, ATSDR is using water-modeling techniques to reconstruct the history of contaminants in the groundwater, in selected water-supply wells, and in the associated water distribution systems. Incorporating models of different levels of complexity as well as those derived from a diversity of perspectives and underlying principles is a sound practice, and one that was recommended by one of the expert panels convened to provide guidance for the Camp Lejeune project (Maslia 2009). The LCM approach is one of several water-modeling techniques used in the overall project. Results from the LCM will be considered and integrated with the results of various other models and approaches to produce estimates and uncertainty bounds for the concentration of contaminants over time in the finished water at USMCB Camp Lejeune.

Two areas of analysis at USMCB Camp Lejeune are discussed in this report: the Tarawa Terrace analysis area, which is used to verify the LCM approach, and the HPLF analysis area, which is the area of current interest for application of the LCM approach (Figure S5.1). Background information is first presented for the HPLF analysis area because it was the impetus for this part of the Camp Lejeune study.

Hadnot Point Landfill (HPLF) Analysis Area

The HPLF analysis area is defined as the area encompassed by and immediately surrounding Installation Restoration (IR) Program Site 82 and storage lot 203 of IR Site 6 (Figure S5.2). Past waste disposal practices in these two areas were the source of groundwater contaminants in the HPLF area. Site investigations and groundwater monitoring initiated in 1986 and continuing through the 1990s identified PCE, TCE, and their associated degradation products as the primary groundwater contaminants in the HPLF analysis area (Environmental Science and Engineering, Inc. 1988; Baker Environmental, Inc. 1993; CH2M HILL, Inc. and Baker Environmental, Inc. 2002). A brief history of IR Sites 6 and 82 as well as a summary of the environmental site investigations and remediation activities conducted at these two sites are contained in Faye et al. (2010). The geohydrologic framework for this area is described in Faye (2012). Depth to groundwater in the landfill area is typically 5 to 15 feet (ft) below ground surface (Faye et al. 2013).

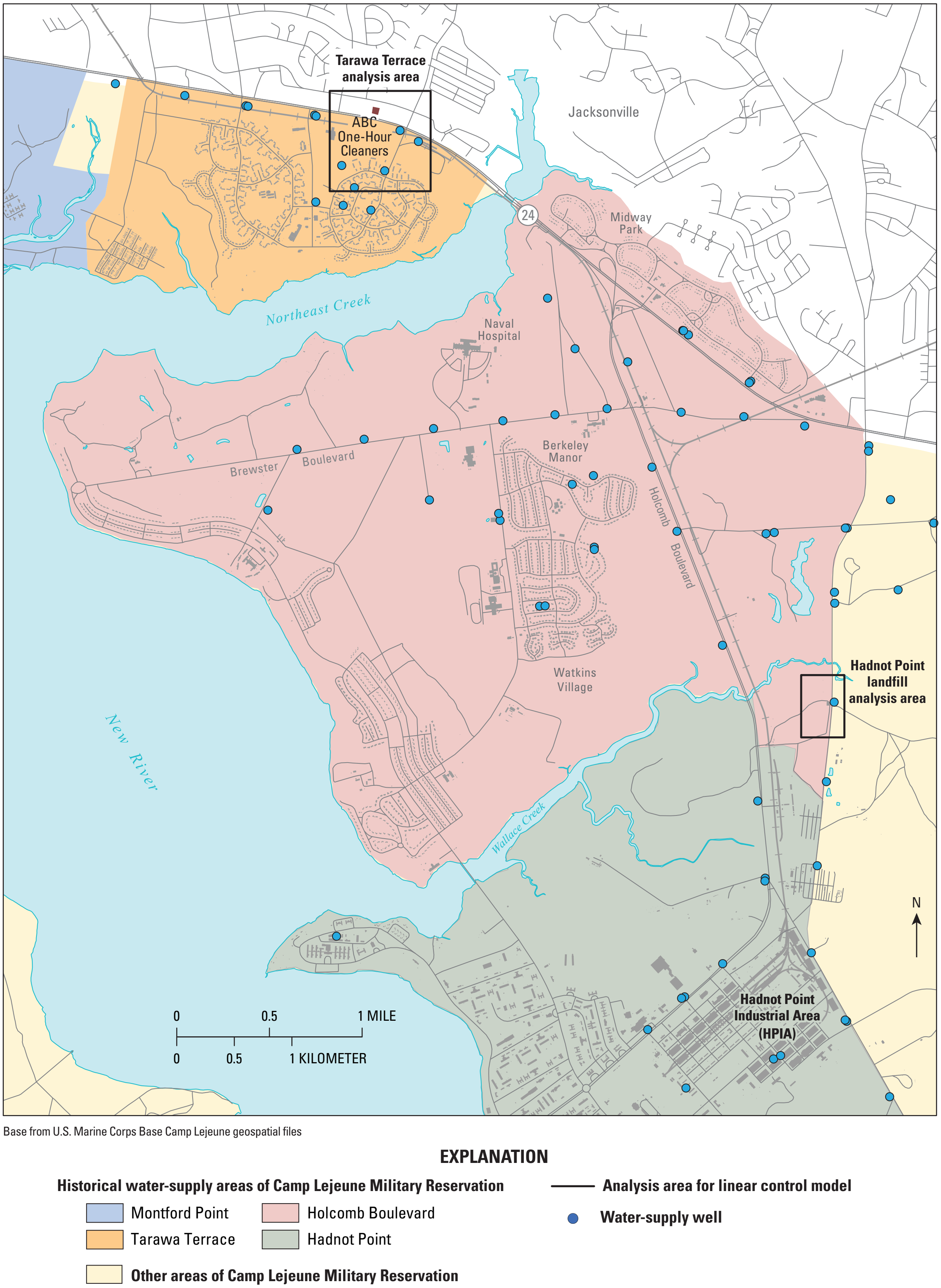
HP-651, located along the eastern side of Sites 6 and 82 (Figure S5.2), is the closest water-supply well to the contaminant source area(s) and the resulting groundwater contaminant plume. High concentrations of TCE (3,200–18,900 μg/L), PCE (307–400 μg/L), and related degradation products were detected in HP-651 during groundwater sampling events in early 1985. As a result, HP-651 was taken out of service on February 4, 1985, and permanently abandoned in June 1994. After HP-651 was shut down, monitor wells were installed in the HPLF area to delineate the horizontal and vertical extent of groundwater contaminants. A groundwater remediation system consisting of 10 remediation wells and a groundwater treatment plant was installed and began operation in January 1996 to remove and treat contaminated groundwater (CH2M HILL, Inc. and Baker Environmental, Inc. 2002).

The service periods for water-supply wells and remediation wells in the HPLF area are illustrated in Figure S5.3. The relative locations of monitor wells and remediation wells in the vicinity of HP-651 are shown in Figures S5.2 and S5.4. The estimated distribution of TCE in groundwater shown in Figure S5.4 is a generalized representation of pre-remediation conditions (1985–1995) for the Upper Castle Hayne aquifer.

The objective for the LCM application for the HPLF analysis area is to reconstruct the history of the contaminants at water-supply well HP-651 for the time period before it was shut down in February 1985. Prior to 1985, no measurements of contaminant concentrations in groundwater are available. Limited data exist from groundwater sampling events at HP-651 conducted in early 1985, 1986 and 1991. Additional contaminant concentration data are available beginning in 1986, when monitoring wells were installed to characterize the nature and extent of groundwater contamination in the area.

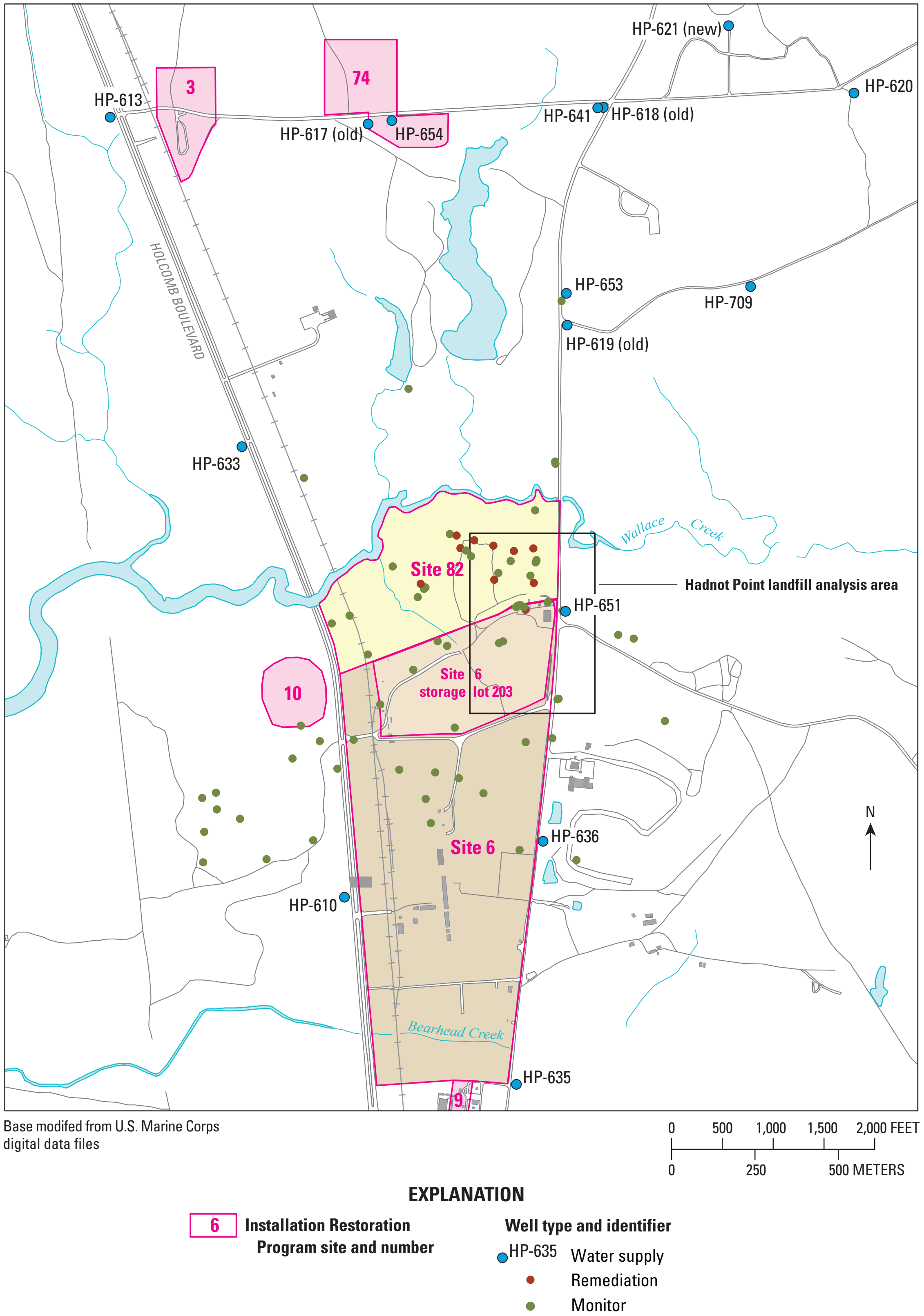
---

[3] For this study, finished water is defined as groundwater that has undergone treatment at a water treatment plant and was subsequently delivered to a family housing unit or other facility. Throughout this report and the Hadnot Point–Holcomb Boulevard report series, the term finished water is used in place of terms such as finished drinking water, drinking water, treated water, or tap water.



Base from U.S. Marine Corps Base Camp Lejeune geospatial files

Figure S5.1. Tarawa Terrace and Hadnot Point landfill analysis and historical water-supply areas, U.S. Marine Corps Base Camp Lejeune, North Carolina.



Base modifed from U.S. Marine Corps digital data files

Figure S5.2. Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

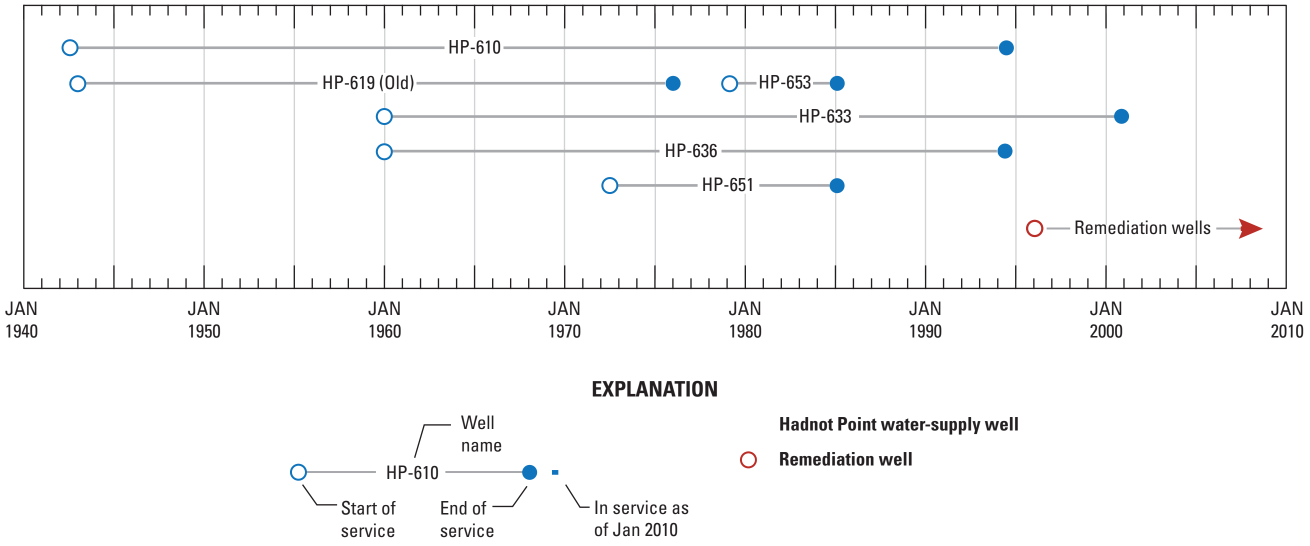
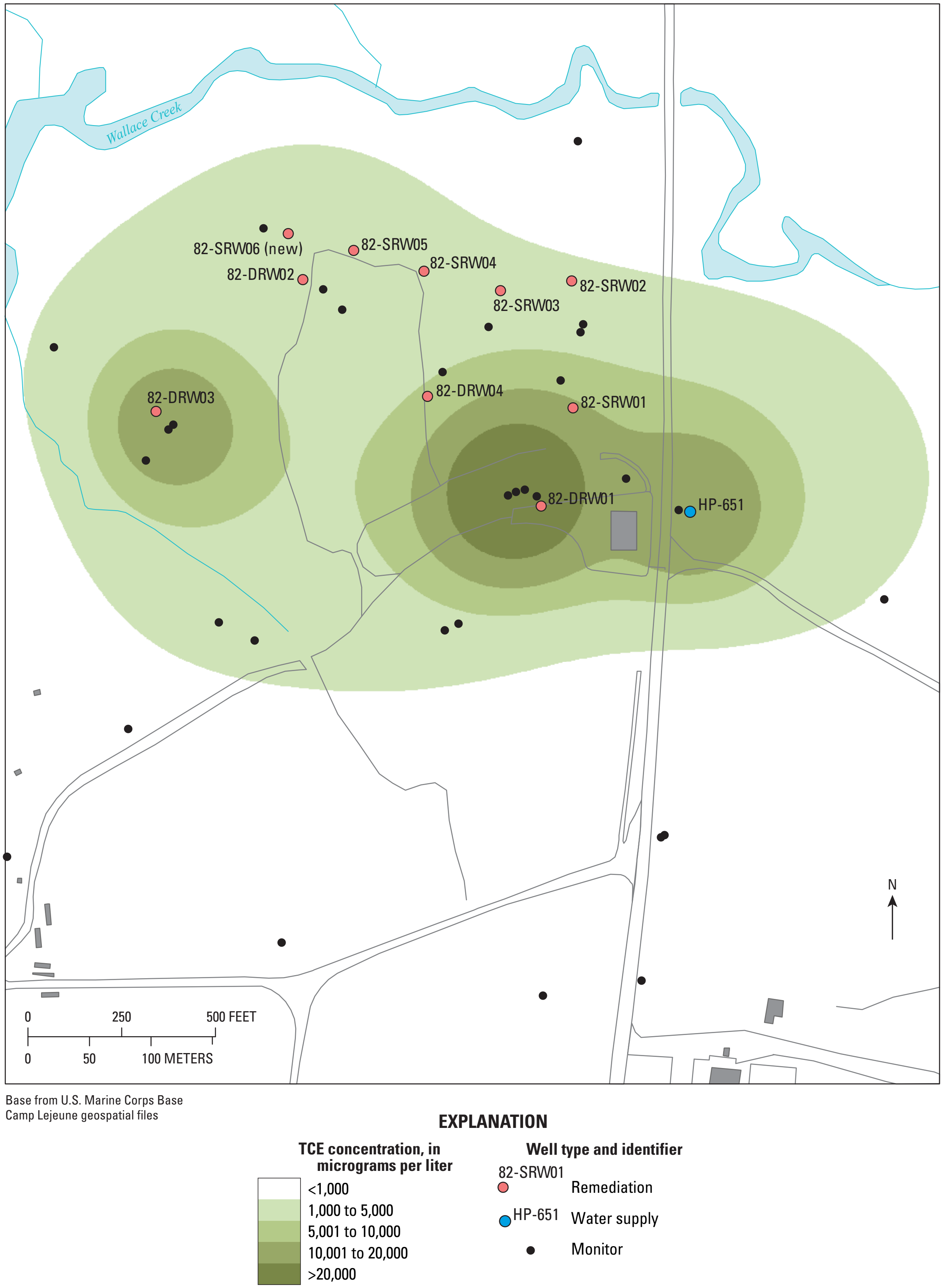


Figure S5.3. Operational chronology of water-supply wells and remediation wells in the Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.



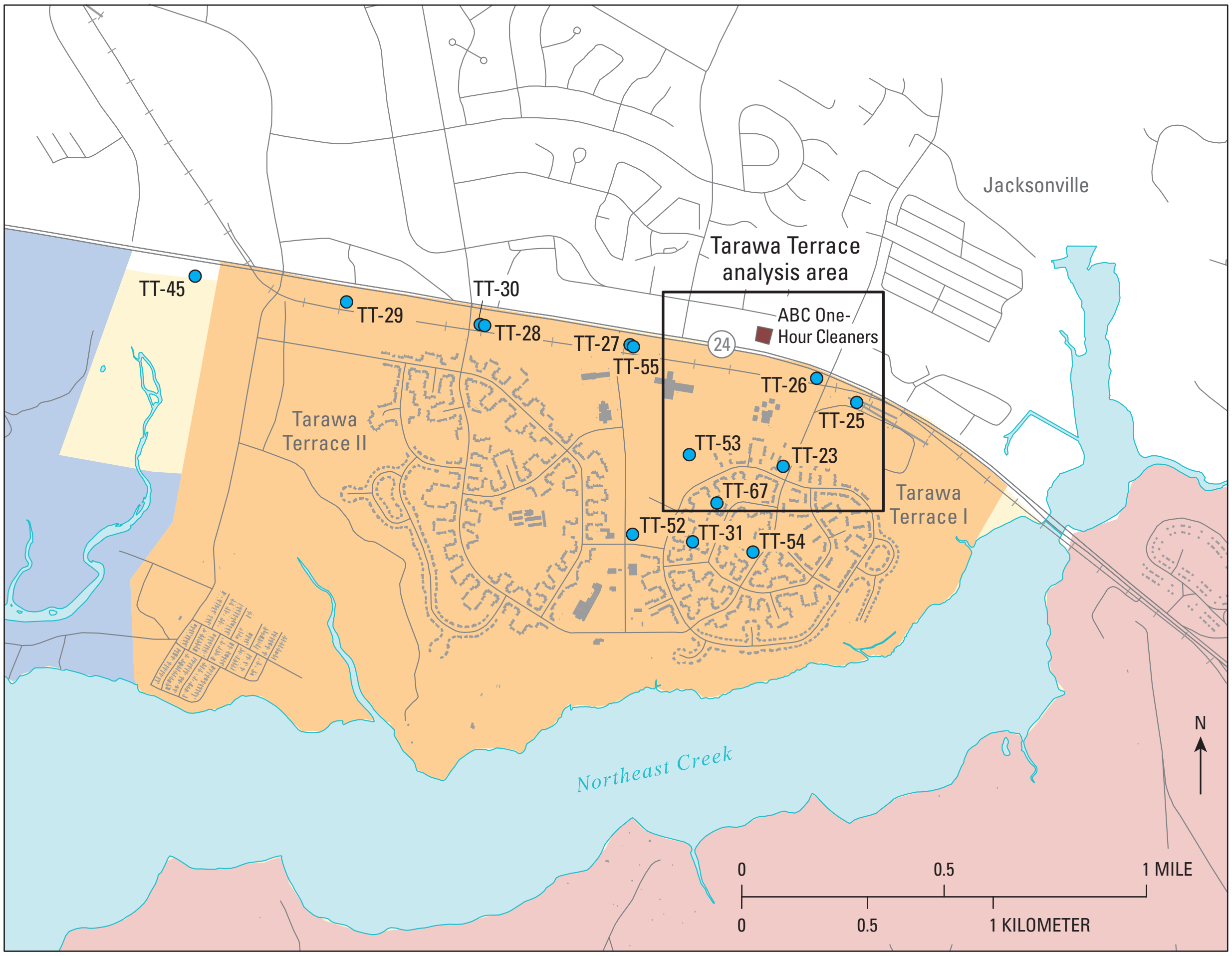
Base from U.S. Marine Corps Base Camp Lejeune geospatial files

Figure S5.4. Water-supply well HP-651 and estimated extent of trichloroethylene (TCE) distribution in the Upper Castle Hayne aquifer, Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina, 1985–1995.

Tarawa Terrace Analysis Area

The Tarawa Terrace analysis area, located on the northern boundary of USMCB Camp Lejeune, includes the Tarawa Terrace family housing area and vicinity (Figure S5.5). Historically, groundwater was the sole source of drinking water for Tarawa Terrace. Fourteen water-supply wells supplied groundwater to the Tarawa Terrace water treatment plant (WTP) and associated water-distribution system. As a result of chlorinated solvent contamination, these water-supply wells were removed from service during 1985–1987, and the Tarawa Terrace WTP was closed in March 1987. Groundwater contamination in this analysis area was linked to the historical release of PCE from a commercial dry cleaning facility, ABC One-Hour Cleaners, located adjacent to USMCB Camp Lejeune (Faye and Green 2007; Maslia et al. 2007).

ATSDR, in partnership with the Georgia Institute of Technology (Georgia Tech) under a cooperative agreement, completed a historical reconstruction of PCE and degradation products in the Tarawa Terrace analysis area of Camp Lejeune using numerical, finite-element methods for modeling groundwater flow and contaminant fate and transport (Maslia et al. 2007; Jang and Aral 2008). Details of the three-dimensional, multispecies, multiphase mass transport model that Georgia Tech developed for the Tarawa Terrace analysis area are provided in Jang and Aral 2008. Synthetic results generated using a modified version of this Tarawa Terrace numerical model are used to verify the LCM approach described herein.



Base from U.S. Marine Corps Base Camp Lejeune geospatial files

EXPLANATION

Historical water-supply areas of Camp Lejeune Military Reservation

🟦 Montford Point
🟥 Holcomb Boulevard
🟧 Tarawa Terrace
🟩 Hadnot Point

🟨 **Other areas of Camp Lejeune Military Reservation**

● TT-54 **Water-supply well and identifier**

Figure S5.5. Tarawa Terrace analysis area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Conceptual Framework for the Linear Control Model (LCM) Approach

The scenario to be modeled can be represented by a generalized sketch of contaminant concentration versus time at two arbitrary observation locations, P1 and P2, within a groundwater aquifer system (Figure S5.6).

For this groundwater aquifer system, the initial time that contaminants are introduced into the groundwater is t_0, the point in time when contaminated water-supply wells at the site are shut down is t_a, and the terminal time for the model is T_f. During Period 1 ($[t_0, t_a]$), the water-supply well(s) are operating (pumping) to withdraw groundwater from the aquifer. During Period 2 ($[t_a, T_f]$), the water-supply wells are not operating (i.e., they are not pumping groundwater from the aquifer). Measured values of contaminant concentration in groundwater are available at selected observation locations during Period 2 (solid lines), but the contaminant history (dashed lines) prior to Period 2 is limited or unavailable and therefore needs to be reconstructed. The reconstruction process uses available water-supply well operational schedules (i.e., pumping rates and operating times) during Period 1 and contaminant concentration data available at selected observation locations during Period 2. The selected locations where contaminant history will be reconstructed may be monitoring wells, water-supply wells, remediation wells, or other features, as long as contaminant concentration data are available at these locations during Period 2.

Notice that the contaminant concentration at time t_a is both the initial value of the concentration for Period 2 and also the outcome or endpoint concentration from Period 1. In other words, at time t_a the contaminant concentration at each observation location is essentially a target “match point” between the time domains spanned by Periods 1 and 2. This is an important component of the solution methodology of the LCM approach that is explained in more detail later.

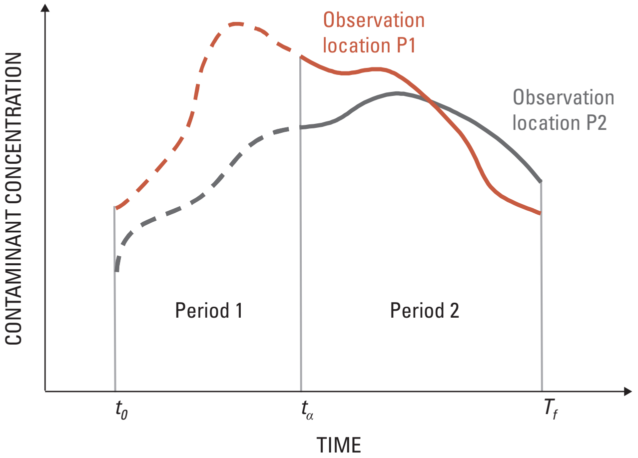


Figure S5.6. Generalized sketch of contaminant concentration versus time in a groundwater aquifer system. [t_0, initial time that contaminants are introduced into the groundwater; t_a, the point in time when contaminated water-supply wells at the site are shut down; T_f, the terminal time for the model]

Limited contaminant data may be available at the observation locations during Period 1. Such data are designated “internal data” or “internal points” because they are within the period during which we are attempting to reconstruct the contaminant history. One would expect that the accuracy of the reconstructed contaminant concentrations during Period 1 would improve if internal data are available. In practice, the availability and quality of internal data are expected to vary. In some cases, internal data may be unavailable.

To summarize, the important components of the conceptual model are as follows.

- Reconstruction of contaminant history occurs at selected observation locations during Period 1.
- Contaminant data must be available during Period 2 at the selected observation locations.
- Operational schedules (i.e., pumping rates and operating times) for water-supply wells in the analysis domain must be available during Period 1.
- Contaminant data at the observation locations may be limited or unavailable during Period 1; if available, these data are designated “internal data” or “internal points.”

The foundation of the LCM approach is derived from control theory principles, which are well-known and well-established in the literature (Aliev and Larin 1998; Pardalos and Yatsenko 2008). Control theory has been widely applied in various fields, including groundwater management (Atwood and Gorelick 1985; Ahlfeld and Heidari 1994; Culver and Shoemaker 1992). In this analysis we simplify the reconstruction of groundwater contamination history as a linear control model based on the available historical data. The LCM approach is a linear state-space representation of the contaminated groundwater aquifer system that includes two system matrices to characterize system behavior. One matrix of the LCM is associated with the movement of the contaminants in the aquifer under natural environmental conditions characterized by little or no groundwater withdrawal from well operations (Period 2 in Figure S5.6). The coefficients of this matrix are developed by applying the least squares method of regression on available field data for contaminant concentrations in groundwater during Period 2. The second matrix of the LCM reflects the effect of water-supply well operations (pumping) on contaminant migration (Period 1 in Figure S5.6). The coefficients of this second system matrix are determined by applying an optimization model that is solved using a modified genetic algorithm (Holland 1975; Guan and Aral 1999).

Reconstruction of contamination history in groundwater using traditional numerical methods is an inverse problem that tends to be mathematically complex and, if it is ill-posed, may be difficult or impossible to solve (Jones et al. 1987; Neupauer et al. 2000; Aral et al. 2001). In this LCM approach, the historical reconstruction problem (i.e., the inverse problem) is transformed into a system characterization problem using the methods adopted from control theory (Aliev and Larin 1998; Pardalos and Yatsenko 2008). The resulting LCM inverse problem is solved using optimization methods.

Methods

In the following subsections, the mathematical underpinnings of the LCM formulation, solution methodology, and uncertainty analysis are described in detail. Subsequently, the methods and framework for LCM verification and application at the HPLF analysis area are outlined.

Mathematical Model Formulation

In the conceptual model introduced previously (Figure S5.6), assume that there are n observation locations (monitor wells, water-supply wells, or remediation wells) where a sufficient number of contaminant concentration measurements are available during Period 2 ($[t_a, T_f]$), m locations where there are pumping wells (water-supply wells or remediation wells), and l contaminant source locations which have released contaminants to the aquifer over time. The contaminant concentrations at the observation locations are represented by the vector $\boldsymbol{X}(t)$: $\boldsymbol{X}(t) = [x_1(t) \quad x_2(t) \quad x_3(t) \quad \dots \quad x_i(t) \quad \dots \quad x_n(t)]^T$, where $x_i(t)$ is the contaminant concentration at location i at time t. The pumping rates at the pumping wells are represented by the vector $\boldsymbol{U}(t)$: $\boldsymbol{U}(t) = [u_1(t) \quad u_2(t) \quad u_3(t) \quad \dots \quad u_j(t) \quad \dots \quad u_m(t)]^T$, where $u_j(t)$ is the pumping rate at the pumping well j at time t. The contaminant concentrations at the contaminant sources are represented as the vector $\boldsymbol{C}(t)$: $\boldsymbol{C}(t) = [c_1(t) \quad c_2(t) \quad c_3(t) \quad \dots \quad c_i(t) \quad \dots \quad c_l(t)]^T$, where $c_i(t)$ is the contaminant concentration at the source i at time t. Using control theory principles, the groundwater aquifer system may be described as a black box model with inputs and outputs as shown in Figure S5.7, where $\dot{\boldsymbol{X}}(t)$ is the time derivative of the contaminant concentration vector $\boldsymbol{X}(t)$. Finding the relations between inputs and outputs of this black box model then becomes essentially an inverse parameter identification problem.

If we assume that a contaminant source or sources were releasing contaminants into the aquifer before remediation began and their release rates are fairly constant, then the contaminant sources can be included in the aquifer system matrices rather than being stated and evaluated as a separate term. In this way, the source characteristics (timing and magnitude) are not explicitly reconstructed, but the addition of contaminant mass is nevertheless represented in the system. Based on our knowledge of the governing equations for groundwater flow and contaminant fate and transport and the methods of numerical solution of these equations, contaminant movement in the aquifer may be approximately described by a linear system given as

$$\left.\begin{aligned}\dot{\boldsymbol{X}}(t) &= \Phi \boldsymbol{X}(t) + \Psi \boldsymbol{U}(t) \\ \boldsymbol{X}(t_0) &= \boldsymbol{X}_0\end{aligned}\right\}, \tag{S5.1}$$

where $\boldsymbol{\Phi}$ is the $(n \times n)$ matrix associated with aquifer parameters and contaminant sources, $\boldsymbol{\Psi}$ is the $(n \times m)$ matrix associated with pumping rates at pumping wells, $\dot{\boldsymbol{X}}(t)$ is the time derivative of the contaminant concentration vector at observation points, and $\boldsymbol{X}_0$ is the initial contaminant concentration vector at the observation locations. This vector can be assumed to be zero if t_0 is considered to be the starting time of contamination at the site. The matrices $\boldsymbol{\Phi}$ and $\boldsymbol{\Psi}$ are unknown and need to be identified using both the available

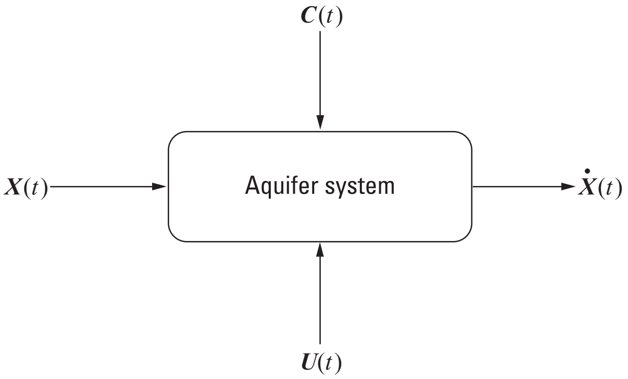


Figure S5.7. Black box model of the groundwater aquifer system. [Variables are defined in preceding text] field data for contaminant concentrations at selected observation locations during Period 2 ($[t_a, T_f]$) and the water-supply well operational records (pumping rate and schedule) during Period 1 ($[t_0, t_a]$). Equation S5.1 will be identified as the system state equation from this point forward.

The system state equation can be solved numerically in the temporal direction. If forward time integration procedures are used, the discretized form of Equation S5.1 becomes

$$\left.\begin{array}{c} \boldsymbol{X}(k+1) = [\boldsymbol{\Phi}\,\Delta t + \mathbf{I}]\,\boldsymbol{X}(k) + \Delta t\,\boldsymbol{\Psi}\,\boldsymbol{U}(k) \\ \boldsymbol{X}(t_0) = \boldsymbol{X}_0 \end{array}\right\}, \qquad \text{(S5.2)}$$

where k is the time step index, Δt is the time step interval, and $\mathbf{I}$ is the identity matrix. For simplicity, let $\mathbf{A} = [\boldsymbol{\Phi}\,\Delta t + \mathbf{I}]$ and let $\mathbf{B} = \boldsymbol{\Psi}\,\Delta t$. Then the discrete system state equation can be given as

$$\left.\begin{array}{c} \boldsymbol{X}(k+1) = \mathbf{A}\boldsymbol{X}(k) + \mathbf{B}\boldsymbol{U}(k) \\ \boldsymbol{X}(t_0) = \boldsymbol{X}_0 \end{array}\right\}. \qquad \text{(S5.3)}$$

Equation S5.3 represents the discrete equation for the numerical solution of the groundwater contaminant transport equations when a forward time integration process is used to solve the problem in the temporal domain. If the terminal states of the system are known, the system state equation may be solved by using a backward time integration process. In this case, the discrete equation can be given by

$$\left.\begin{array}{c} \boldsymbol{X}(k) = \mathbf{A}^{-1}\boldsymbol{X}(k+1) - \mathbf{A}^{-1}\mathbf{B}\boldsymbol{U}(k) \\ \boldsymbol{X}(T_f) = \boldsymbol{X}_f \end{array}\right\}. \qquad \text{(S5.4)}$$

If we define $\mathbf{A}_b = \mathbf{A}^{-1}$; $\mathbf{B}_b = -\mathbf{A}^{-1}\,\mathbf{B}$, then the discrete form of the backward solution of the system state equation can be written as

$$\left.\begin{array}{c} \boldsymbol{X}(k) = \mathbf{A}_b\,\boldsymbol{X}(k+1) + \mathbf{B}_b\boldsymbol{U}(k) \\ \boldsymbol{X}(T_f) = \boldsymbol{X}_f \end{array}\right\}. \qquad \text{(S5.5)}$$

No matter how the time integration of the system equation is performed (forward or backward) during the reconstruction of the contamination history at a site, the coefficients of the system matrices **A** (or $\mathbf{A}_b$) and the coefficients of the matrices related to the pumping terms **B** (or $\mathbf{B}_b$) need to be identified. The identification of the coefficients of the matrices $\mathbf{A}_b$ and $\mathbf{B}_b$ is the same as that of the matrices **A** and **B** in the proposed methodology. Thus, in order to avoid repetition, the discrete forward time integration form of the system state equation will be used in the next section to describe the procedures used in estimating the coefficients of these matrices.

Solution Methodology

Identifying the coefficients of the matrices **A** and **B** is a two-step process. In the first step, the coefficients of matrix **A** are identified by applying the method of least squares to fit a regression model to field data consisting of measured contaminant concentrations at selected observation locations within the period $[t_a, T_f]$. In the second step, the coefficients of the matrix **B** are identified with an optimization method that uses the water-supply well operational data available for Period 1 ($[t_0, t_a]$) combined with contaminant concentrations observed at time t_a.

***Identification of the coefficients of the matrix* A:** If little or no groundwater well pumping is occurring at the site after time t_a, the system state Equation S5.3 for Period 2 ($[t_a, T_f]$) can be written as

$$\boldsymbol{X}(k+1) = \mathbf{A}\,\boldsymbol{X}(k). \qquad \text{(S5.6)}$$

The contaminant concentration state at an observation location i in Equation S5.6 can be written as

$$x_i\left(k+1\right)=\sum_{j=1}^{n} a_{ij} x_j\left(k\right), \qquad i=1,2,3,\cdots,n. \tag{S5.7}$$

where a_{ij} is an element of the matrix **A** in row i and column j. In vector notation, considering all observation points, Equation S5.7 can be written as

$$\left\{x_i\left(k+1\right)\right\}=\left\{x_1\left(k\right) \quad x_2\left(k\right) \quad \ldots \quad x_j\left(k\right) \quad \ldots \quad x_n\left(k\right)\right\}\begin{Bmatrix} a_{i1} \\ a_{i2} \\ \vdots \\ a_{ij} \\ \vdots \\ a_{in} \end{Bmatrix}, \quad i=1,2,3,\ldots,n. \tag{S5.8}$$

In Equation S5.8, it is assumed that Period 2 ($[t_a, T_f]$) is discretized into T time steps, denoted as $k = 1$, 2, 3, , T. For all k, the equation given above can be expressed in matrix notation as

$$\boldsymbol{Y}_i = \boldsymbol{\Lambda} \boldsymbol{a}_i \tag{S5.9}$$

where $\boldsymbol{Y}_i = [\, x_i(1) \quad x_i(2) \quad x_i(3) \quad \ldots \quad x_i(T)]^T$, $\boldsymbol{a}_i = [a_{i1} \quad a_{i2} \;\; a_{i3} \quad \ldots \quad a_{in}]^T$, and the matrix $\boldsymbol{\Lambda}$ is the $T \times n$ matrix defined as

$$\Lambda=\begin{bmatrix} x_1\left(0\right) & x_2\left(0\right) & \cdots & x_n\left(0\right) \\ x_1\left(1\right) & x_2\left(1\right) & \cdots & x_n\left(1\right) \\ \vdots & \vdots & \vdots & \vdots \\ x_1\left(T-1\right) & x_2\left(T-1\right) & \cdots & x_n\left(T-1\right) \end{bmatrix}. \tag{S5.10}$$

Using the least squares method, the parameters $\boldsymbol{a}_i$, represented as $\widehat{\boldsymbol{a}_i}$ (Björck 1996) can be estimated. This process can be represented by

$$\widehat{\boldsymbol{a}_i}=\left(\Lambda^T\Lambda\right)^{-1}\Lambda^T\boldsymbol{Y}_i, \qquad i=1,2,3,\ldots,n\,, \tag{S5.11}$$

where the symbol $\widehat{\ }$ indicates the estimated value. Defining $\widehat{\mathbf{A}}=\left[\widehat{\boldsymbol{a}_1} \quad \widehat{\boldsymbol{a}_2} \quad \widehat{\boldsymbol{a}_3} \quad \ldots \quad \widehat{\boldsymbol{a}_n}\right]^T$ and $\mathbf{Y}=[\boldsymbol{Y}_1 \quad \boldsymbol{Y}_2 \quad \boldsymbol{Y}_3 \quad \ldots \quad \boldsymbol{Y}_n\,]$, then the matrix $\widehat{\mathbf{A}}$ can be estimated by

$$\widehat{\mathbf{A}}=\left[\left(\Lambda^T\Lambda\right)^{-1}\Lambda^T\boldsymbol{Y}\right]^T. \tag{S5.12}$$

The coefficients of the matrix $\widehat{\mathbf{A}}$ estimated above reflect the aquifer characteristics of the site, including the contaminant sources under natural conditions, i.e. without the effects of groundwater well pumping on contaminant migration. The contaminant concentration time series for Period 2 ($[t_a, T_f]$) can be calculated in the forward temporal direction by the use of the discrete state equation as

$$\left.\begin{aligned} \boldsymbol{X}\ \ k+1) &= \widehat{\mathbf{A}}\boldsymbol{X}\left(k\right) \\ \boldsymbol{X}\left(T_0\right) &= \boldsymbol{X}_{T_0} \end{aligned}\right\}, \tag{S5.13}$$

where T_0 is any point in the interval $[t_a, T_f]$.

Identification of the coefficients of the matrix* B*: Because contaminant concentration data may be unavailable during Period 1 ($[t_0, t_a]$), the method described above cannot be used to estimate the coefficients of the matrix **B**. However, notice that the contaminant concentrations at observation points at time t_a are not only the initial values of concentration for Period 2 ($[t_a, T_f]$) but also the outcome or endpoint concentrations of the pumping operations during Period 1 ($[t_0, t_a]$). At time t_a the contaminant concentration at each observation location is essentially a target "match point" between the time domains spanned by matrix **A** and matrix **B**. Using the contaminant concentration data at time t_a, estimation of the coefficients of the matrix **B** may be formulated as an optimization problem. By applying an optimization model and minimizing total error between the estimated and observed contaminant concentrations at time t_a, based on an estimated $[t_0, t_a]$ time interval solution of the system equation, the coefficients of the matrix **B** can be determined. The optimization model can be mathematically stated as

$$\left.\begin{array}{l} f = \min\limits_{\mathbf{B}} \left\{ \dfrac{1}{2} \sum\limits_{i=1}^{n} \left(x_i(t_a) - x_i^*(t_a) \right)^2 \right\} \\ \\ \textit{subject to}: \\ \quad \boldsymbol{X}(k+1) = \widehat{\mathbf{A}}\boldsymbol{X}(k) + \widehat{\mathbf{B}}\boldsymbol{U}(k) \\ \quad \boldsymbol{X}(k) \geq 0 \\ \quad \boldsymbol{X}(t_0) = 0 \end{array}\right\}, \tag{S5.14}$$

where f is the objective function, $x_i(t_a)$ is the estimated contaminant concentration at the observation location i at time t_a, which is obtained from the solution of the system state Equation S5.3, $x_i^*(t_a)$ is the observed contaminant concentration at the monitoring location i at time t_a, and

$$\begin{array}{l} \boldsymbol{X}(k+1) = \widehat{\mathbf{A}}\boldsymbol{X}(k) + \widehat{\mathbf{B}}\boldsymbol{U}(k) \\ \boldsymbol{X}(t_0) = 0 \end{array}, \tag{S5.15}$$

is the approximate form of the of the discrete system Equation S5.3. Because the coefficients of the matrix $\widehat{\mathbf{A}}$ are already determined during the previous step, in the optimization model, the parameters $x_i(t_a)$ are a function of the coefficients of the matrix $\widehat{\mathbf{B}}$ that will be determined.

If there are some internal contaminant concentration data available at the observation locations during Period 1 ($[t_0, t_a]$), whose time step index set for the observation site i is denoted as $\boldsymbol{P}(i)$, then this information can also be used to improve the estimates of the coefficients of the matrix **B**. For this case, the objective function used in Equation S5.14 can be given as:

$$f = \min_{\mathbf{B}} \left\{ \frac{1}{2} \left[\sum_{i=1}^{n} \left(x_i(t_a) - x_i^*(t_a) \right)^2 + \sum_{i=1}^{n} \sum_{l \in \boldsymbol{P}(i)} \left(x_i(l) - x_i^*(l) \right)^2 \right] \right\}. \tag{S5.16}$$

In Equation S5.16, l indicates the time step index in $\boldsymbol{P}(i)$ for internal data that is available for the observation location i. If there are no internal data (i.e., contaminant concentration data during Period 1 ($[t_0, t_a]$) for site i), then $\boldsymbol{P}(i)$ is an empty set. The optimization model described above may be solved by using a genetic algorithm.

Genetic algorithms (GAs) are novel heuristic search techniques that are based on the mechanics of natural selection and natural genetics, combining artificial survival of the fittest concepts with genetic operations abstracted from nature (Holland 1975). Since their initiation in 1975, GAs have been widely applied in numerous fields, including groundwater resources management (Guan and Aral 1999; Guan et al. 2007). The principles and procedures of GAs can be found in the literature (Holland 1975; Guan and Aral 1999) and will not be repeated here. Typically, when GAs are used to solve an optimization problem, the bounds of the unknown variables are known. However, in the LCM model for this analysis, the ranges of the coefficients of the matrix **B**, b_{ij}, are unknown. Although the ranges can be specified artificially, such arbitrary choices will affect the accuracy of the solution and the computation time. If the selected range is too large, the computational time will increase significantly. If the selected range is too small, the optimal solution may, in fact, lie outside of the selected range. To resolve this issue, a modified genetic algorithm is proposed based on the sub-domain concept and the iteration mechanism proposed by Guan and Aral (1999). The basic steps of this approach are as follows:

1. Select an initial "corridor" for the identified parameters, expressed as

$$-\Delta b_{ij}^{(0)} \le b_{ij} \le +\Delta b_{ij}^{(0)}; \forall i, j \,, \qquad \text{(S5.17)}$$

   where $\Delta b_{ij}^{(0)}$ is the width of the initial corridor.

2. Apply the standard genetic algorithm procedures to find the best solution within the corridor, denoted as b_{ij}^{*}.

3. Specify a new corridor based on the best solution:

$$b_{ij}^{*} - \Delta b_{ij}^{(l)} \le b_{ij} \le b_{ij}^{*} + \Delta b_{ij}^{(l)}; \ \forall i, j \,, \qquad \text{(S5.18)}$$

   where $\Delta b_{ij}^{(l)}$ is the width of the corridor in the lth iteration, which should decrease as iterations improve. For example, $\Delta b_{ij}^{(l)}$ may be set as

$$\Delta b_{ij}^{(l)} = \Delta b_{ij}^{(0)} e^{-\gamma l} \,, \qquad \text{(S5.19)}$$

   where γ is a contraction coefficient. Accordingly, as iteration progresses, the width of the corridor gradually reduces. In the next iteration, the best solution of the last iterative step should be a member of the initial population of the next step for the iteration process to converge monotonically.

4. Repeat steps 1–3 until the best solutions obtained in two consecutive iterations satisfy the selected allowable error or until the iteration reaches a given maximum number of iterations selected as the stopping criteria. The final best solutions are taken as the estimated value of b_{ij}, denoted as $\hat{b}_{ij}$.

In summary, the two-step procedure for the identification of the discrete system state equation can be illustrated by the flowchart shown in Figure S5.8.

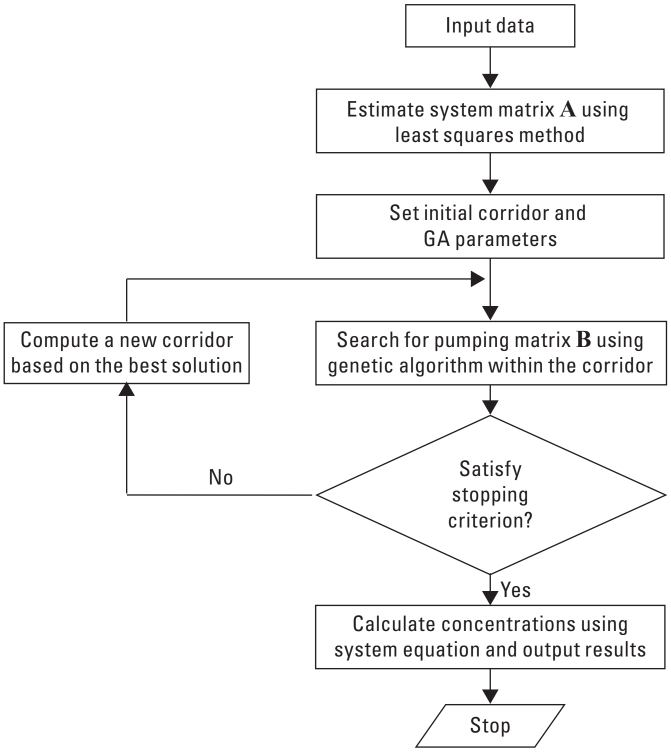


Figure S5.8. Flowchart for identification of the matrix coefficients of the discrete system state equation. [GA, genetic algorithm]

Uncertainty Analysis for Modeling and Measurement Errors

The LCM system state equations, Equations S5.3 and S5.5, are deterministic in nature and therefore do not incorporate numerical errors that may originate from modeling or measurement errors from field data collection efforts. Numerical errors propagate in the system and directly affect the reconstruction of contaminant history. A Kalman filter can incorporate error propagation in dynamic systems (Zhou and van Geeralmod 1992). Therefore, to analyze the effect of such errors on the contaminant concentration distributions that are reconstructed, a Kalman filter is coupled with Monte Carlo simulation in this application. The confidence corridor of contaminant concentration distributions at observation locations is constructed using the statistical interpretation for a given confidence level. As was done previously, the model and algorithms developed in this section will focus only on the forward time integration form of the discrete system state equation, Equation S5.3.

Kalman Filter Algorithm Coupled with Monte Carlo Simulation

The system state equation with system error incorporated is stated mathematically as

$$\boldsymbol{X}(k) = \mathbf{A}\boldsymbol{X}(k-1) + \mathbf{B}\boldsymbol{U}(k-1) + \boldsymbol{w}(k), \qquad \text{(S5.20)}$$

and the measurement equation is given as

$$\boldsymbol{Y}(k) = \mathbf{C}\boldsymbol{X}(k) + \boldsymbol{v}(k), \qquad \text{(S5.21)}$$

where **A** and **B** are the system and pumping effect matrices identified earlier, $\boldsymbol{w}(k)$ is the system noise at stress period k, $\boldsymbol{Y}(k)$ is the contaminant concentration measurement at time step k, **C** is the concentration measurement matrix at time step k, and $\boldsymbol{v}(k)$ is the measurement error vector at time step k. The system error and the measurement error are assumed to be multidimensional, homogenous, zero-mean Gaussian processes. The Kalman filter algorithm is given by the following equations:

$$\begin{aligned}
&\bar{\boldsymbol{X}}(k) = \mathbf{A}\widehat{\boldsymbol{X}}(k-1) + \mathbf{B}\boldsymbol{U}(k-1)\\
&\mathbf{M}(k) = \mathbf{A}\mathbf{P}(k)\mathbf{A}^T + \mathbf{Q}(k)\\
&\mathbf{K}(k) = \mathbf{M}(k)\mathbf{C}^T[\mathbf{C}\mathbf{M}(k)\mathbf{C}^T + \mathbf{R}(k)]^{-1}\\
&\widehat{\boldsymbol{X}}(k) = \bar{\boldsymbol{X}}(k) + \mathbf{K}(k)[\boldsymbol{Y}(k) - \mathbf{C}\bar{\boldsymbol{X}}(k)]\\
&\mathbf{P}(k) = [\mathbf{I} - \mathbf{K}(k)\mathbf{C}]\mathbf{M}(k)
\end{aligned} \qquad \text{(S5.22)}$$

,

where $\widehat{\boldsymbol{X}}(k)$ is the measurement-updated concentration at time step k; $\bar{\boldsymbol{X}}(k)$ is the time-updated concentration at time step k; $\mathbf{P}(k)$ is the covariance matrix of the error of the measurement-updated concentration, $\mathrm{cov}\{\boldsymbol{X}_k - \widehat{\boldsymbol{X}}_k\}$; $\mathbf{M}(k)$ is the covariance matrix of the error of the time-updated concentration, $\mathrm{cov}\{\boldsymbol{X}_k - \bar{\boldsymbol{X}}_k\}$; $\mathbf{Q}(k)$ is the covariance matrix of the system noise; $\mathbf{R}(k)$ is the covariance matrix of the measurement error; $\mathbf{K}(k)$ is the Kalman gain matrix; and **I** is the identity matrix. In the reconstruction problem, **Q** and **R** are assumed to be independent of time, and **C** is an identity matrix. Thus, the Kalman filter algorithm can be simplified as

$$\begin{aligned}
&\bar{\boldsymbol{X}}(k) = \mathbf{A}\widehat{\boldsymbol{X}}(k-1) + \mathbf{B}\boldsymbol{U}(k-1)\\
&\mathbf{M}(k) = \mathbf{A}\mathbf{P}(k)\mathbf{A}^T + \mathbf{Q}\\
&\mathbf{K}(k) = \mathbf{M}(k)[\mathbf{M}(k) + \mathbf{R}]^{-1}\\
&\widehat{\boldsymbol{X}}(k) = \bar{\boldsymbol{X}}(k) + \mathbf{K}(k)[\boldsymbol{Y}(k) - \bar{\boldsymbol{X}}(k)]\\
&\mathbf{P}(k) = [\mathbf{I} - \mathbf{K}(k)]\mathbf{M}(k)
\end{aligned} \qquad \text{(S5.23)}$$

.

In order to apply the Kalman filter algorithm to reconstruction of contamination history, the system noise, expected measurement error, and contaminant concentration measurements must be determined.

System Noise

The system noise represents all unknown error, including modeling error and uncertainties in system parameters. Based on the assumption of the Kalman filter algorithm, the system noise can be completely described by the covariance matrix **Q**. The covariance of the system noise may be expressed as

$$q_{i,j} = \sigma_i \sigma_j \rho(l)\,, \qquad \text{(S5.24)}$$

where σ_i and σ_j are the standard deviations of the system noise at observation locations i and j, l is the distance between observation locations i and j, and $\rho(l)$ is the correlation coefficient of the system noise at separation l. The standard deviation of the system noise can be estimated from measured concentrations used to identify system matrix **A** and the concentrations reconstructed from the system state equation without the pumping effect term. The correlation coefficient of the system noise represents the spatial coherence between the corresponding observation locations. It reflects the spatial effect of concentration at one location in reference to the concentrations at other locations. Obviously, the closer the corresponding locations are, the larger their correlation coefficient is. Three correlation models have been proven to be useful to characterize the system noise.

An exponential correlation model is defined as

$$\rho(l) = \exp(-l/a)\,, \qquad \text{(S5.25)}$$

where a is a parameter indicating the magnitude of the spatial correlation and can be estimated by the spatial correlation length, l_c, defined as

$$l_c = \int_0^\infty \rho(l)\,dl\,, \qquad \text{(S5.26)}$$

then $a = l_c$.

A Gaussian correlation model is defined as

$$\rho(l) = \exp(-(l/b)^2) , \qquad \text{(S5.27)}$$

where *b* is a parameter indicating the magnitude of the spatial correlation and can be estimated by

$$b = l_c / \sqrt{\pi / 2} . \qquad \text{(S5.28)}$$

A spherical correlation model is defined as

$$\rho(l) = \begin{cases} 1 - 1.5(l/\lambda) + 0.5(l/\lambda)^3, & l < \lambda \\ 0 & l > \lambda \end{cases} , \qquad \text{(S5.29)}$$

where λ is a parameter indicating the magnitude of the spatial correlation and can be estimated by

$$\lambda = 8l_c / 3 , \qquad \text{(S5.30)}$$

The changes in spatial correlation with each of these three correlation models are shown in Figure S5.9. Overall, the correlation coefficient decreases as the distance between observation locations increases, although there are differences in the rate of decrease for each model.

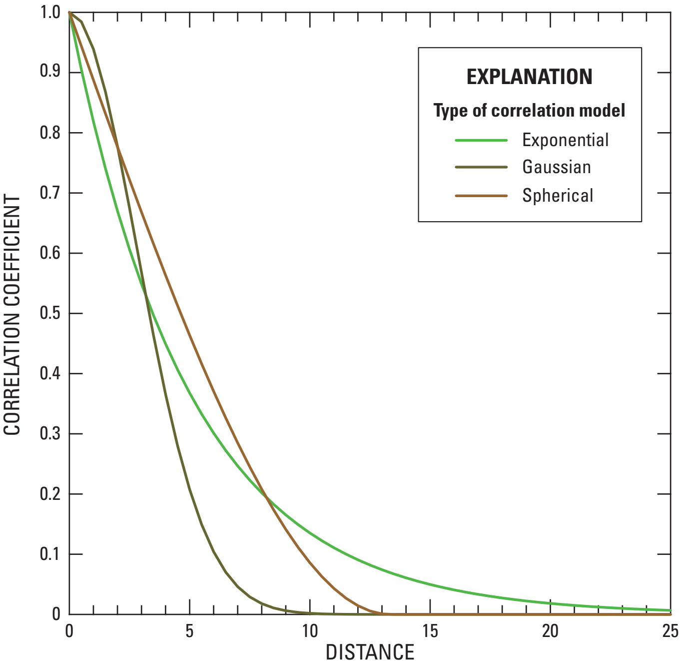


Figure S5.9. Comparison of correlation models with correlation length of 5.

Measurement Error

The measurement errors are assumed to be independent random variables with zero mean. Thus, the covariance matrix of measurement error is defined as a diagonal matrix given as

$$\boldsymbol{R} = diag\{\sigma_{r_1}^2, \sigma_{r_2}^2, \ldots, \sigma_{r_n}^2\} , \qquad \text{(S5.31)}$$

where $\sigma_{r_i}^2$ is the variance of measurement error at site *i*. The variance depends on the accuracy of the measurement equipment used and is generally assumed to be known. In this analysis we have defined this error to be constant at all measurement locations, i.e., $\sigma_{r_1}^2 = \cdots = \sigma_{r_n}^2 = \sigma_r^2 = \text{constant}$.

Measurements of Contaminant Concentration

The Kalman filter algorithm requires some measurements of contaminant concentration ***Y(k)***. Because the purpose of this analysis is to reconstruct the contaminant concentration distributions at observation locations, measurements of contaminant concentration are not available during Period 1 ($[t_0, t_a]$).

To resolve this issue, Monte Carlo simulation is used to generate contaminant concentration values based on the LCM approach. The procedure for implementing the Monte Carlo simulation can be described as follows:

1. The LCM is used to reconstruct concentration distributions at observation locations.
2. The Monte Carlo simulation is used to generate n_{mc} sets of random series with normal distribution characterized by zero mean and a variance given in measurement error (Skaggs and Kabala, 1994). The necessary measurements of contaminant concentrations may then be defined as

   $$y_i(k) = x_i(k) + \varepsilon_i(k)\beta_i , \qquad \text{(S5.32)}$$

   where n_{mc} is the number of Monte Carlo simulations, $\varepsilon_i(k)$ is the random number generated, and β_i is the strength of error at site *i*.
3. The Kalman filter algorithm is used to obtain the smooth solutions.
4. Statistical analysis on the smooth solutions yields the probability distribution at each time step for all observation locations. The average, maximum, and minimum concentration distributions as well as probability distribution at each time step for each observation location may be obtained, as shown in Figure S5.10. Furthermore, the confidence intervals, or "corridors," of concentration distributions at observation locations can also be obtained for the given confidence level selected.

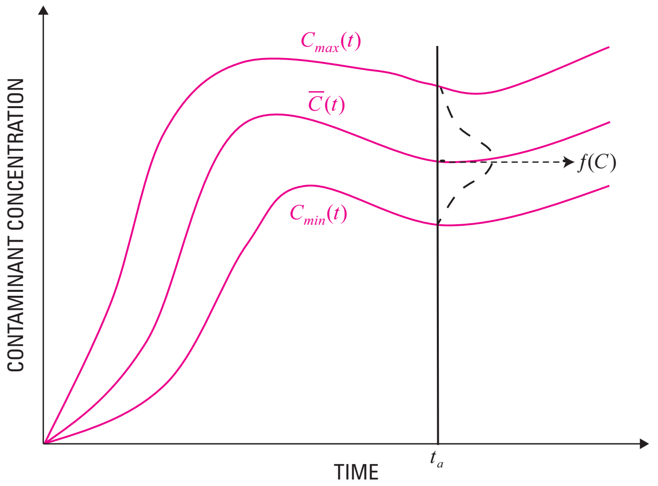


Figure S5.10. Illustration of Monte Carlo simulation results. [$C_{min}(t)$, $C_{max}(t)$, and $\overline{C}(t)$ are the minimum, maximum, and mean contaminant concentrations, respectively, at time t at an observation location; $f(C)$, the probability density function of the concentration; t_a, an arbitrary point in time]

Estimation of Confidence Intervals

Based on the results of the Monte Carlo simulation, the confidence interval on the mean contaminant concentration at observation locations can be estimated for a normal distribution at a given confidence level α using statistical methods. The mean and standard deviation of contaminant concentrations at each stress period and observation location can be calculated by

$$\overline{x}_i(t) = \frac{1}{n_{mc}} \sum_{m=1}^{n_{mc}} x_i^m(t), \qquad \text{(S5.33)}$$

and

$$s_i(t) = \sqrt{\frac{1}{n_{mc}-1} \sum_{m=1}^{n_{mc}} (x_i^m(t) - \overline{x}_i(t))^2}, \qquad \text{(S5.34)}$$

where n_{mc} is the number of Monte Carlo simulations, $x_i^m(t)$ is the contaminant concentration at observation location i at stress period t in the m^{th} Monte Carlo simulation, $\overline{x}_i(t)$ is the mean of the contaminant concentration at observation location i at stress period t, and $s_i(t)$ is the standard deviation of the contaminant concentration at observation location i at stress period t.

For a normal distribution, at a given confidence level α, the confidence interval can be estimated by

$$\overline{x}_i(t) - t_{\alpha/2, n_{mc}-1} \frac{s_i(t)}{\sqrt{n}} \le x_i(t) \le \overline{x}_i(t) + t_{\alpha/2, n_{mc}-1} \frac{s_i(t)}{\sqrt{n}}, \qquad \text{(S5.35)}$$

where $t_{\alpha/2, n_{mc}-1}$ is the t-distribution with (n_{mc} − 1) degree of freedom.

If the concentrations at each stress period do not follow a normal distribution, a confidence interval that represents a percentile range of the Monte Carlo results may be calculated (Walpole et al. 2007). Because we do not know whether the Monte Carlo results follow a normal distribution, the percentile range method is used to calculate the confidence interval. The procedure used for this calculation is as follows:

1. For each stress period and each observation site, find the minimum and maximum values of the contaminant concentration and divide the range into n_h sub-intervals;
2. Calculate the corresponding frequencies for each sub-interval (f_i);
3. Assume the distribution is symmetric. For a given confidence level α, perform the summation calculation

$$p_1 = \sum_{i=1}^{l_1 \le n_h} f_i \text{ and } p_2 = \sum_{i=n_h}^{l_2 \ge 1} f_i, \qquad \text{(S5.36)}$$

until $p_1 \ge \frac{\alpha}{2}$ or $p_2 \ge \frac{\alpha}{2}$, as shown in Figure S5.11.

In Equation (S5.36), n_h is the number of sub-intervals given, l_1 is the index of the sub-interval in which $p_1 \ge \frac{\alpha}{2}$, l_2 is the index of the sub-interval in which $p_2 \ge \frac{\alpha}{2}$, and p_1 and p_2 are the cumulative probabilities in left side and right side. The corresponding contaminant concentration at interval l_1 is taken as the lower bound of the confidence interval. Likewise, the contaminant concentration at interval l_2 is taken as the upper bound of the confidence interval.

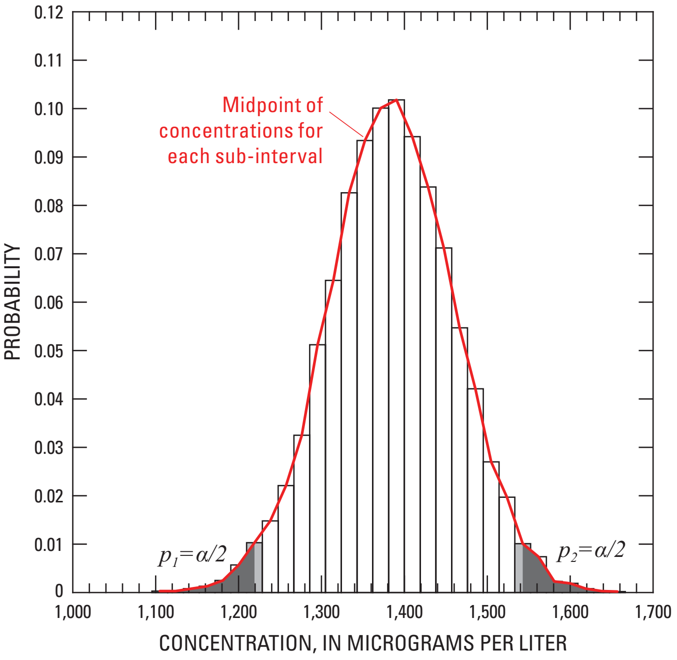


Figure S5.11. Illustration of confidence intervals from a histogram for a given α.

LCM Verification Using the Tarawa Terrace Numerical Model

For the purposes of the LCM verification, the aquifer parameters, boundary conditions, and source characteristics of the Tarawa Terrace numerical model are the same as those defined in the previous analysis (Jang and Aral 2008). Based on the results of the previous analysis, 3 of the 14 water-supply wells in the model had a significant effect on contaminant migration in the area. To simplify the system, only these three water-supply wells—TT-26, TT-53, and TT-67—are included in the current Tarawa Terrace simulations for LCM verification. The end-of-service for TT-53 is December 1983, while the end-of-service for TT-26 and TT-67 is programmed for this analysis to be the end of December 1984[4], which mimics the shutdown date of water-supply well HP-651 in the HPLF analysis area. The historical operating schedules for these three Tarawa Terrace water-supply wells (Figure S5.12) correspond to the calibrated pumping schedule presented in Faye and Valenzuela (2007), which is also referred to as the "Original Pumping Schedule" (PS-O) in several companion reports (Jang and Aral 2008; Wang and Aral 2008).

Using this modified Tarawa Terrace numerical model, simulated PCE concentrations in groundwater are generated for five selected observation locations. These five observation locations correspond to water-supply well TT-26 and four other nodes of the Tarawa Terrace model grid (Table S5.1, Figure S5.13) that are distributed within the simulated PCE groundwater plume emanating from the contaminant source (ABC One-Hour Cleaners). Simulated results for PCE concentration in groundwater during January 1951–December 1994 at each of these five locations are shown in Figure S5.14. Note that water-supply wells TT-26, TT-53, and TT-67 are shut down at the end of December 1984 in the model simulation.

In the verification task, both the forward and backward time integration formulations of the LCM approach are evaluated using the synthetic results from the modified TT model. The simulated PCE results during Period 2 (December 1984–December 1994) are used to determine the coefficients of the system matrix $\widehat{\mathbf{A}}$ using the method of least squares and the appropriate forward or backward time integration form of the system state equation (e.g., Equation S5.13). The water-supply well schedules during Period 1 (Figure S5.12) and PCE concentration for December 1984 (the "match point" of Period 1 and Period 2) are used to identify the coefficients of matrix $\widehat{\mathbf{B}}$ using the genetic algorithm approach and the appropriate forward or backward time integration form of the system state equation (e.g., Equation S5.15).

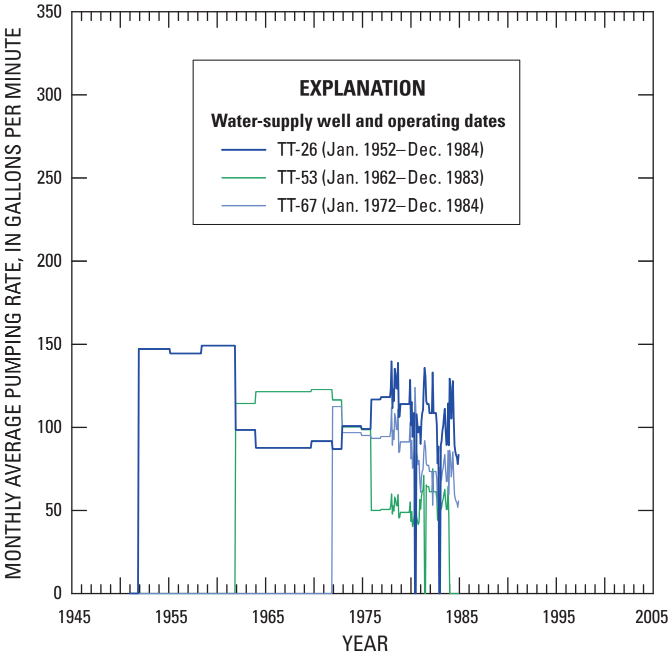


Figure S5.12. Operational schedule for selected water-supply wells in the Tarawa Terrace analysis area, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.5 for well locations]

Table S5.1. Observation locations for Tarawa Terrace simulations, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NC SPCS, North Carolina State Plane Coordinate System]

Observation location[1]	Tarawa Terrace model node[2]	Easting coordinate, in feet NC SPCS[3]	Northing coordinate, in feet NC SPCS[3]	Altitude, in feet below land surface
1	102570	2,491,519	364,045	80
2	103438	2,491,509	364,230	80
3, TT-26[4]	103860	2,491,461	364,656	90–108
4	104066	2,491,252	364,379	80
5	104892	2,490,867	364,560	80

[1] See Figure S5.13 for observation locations

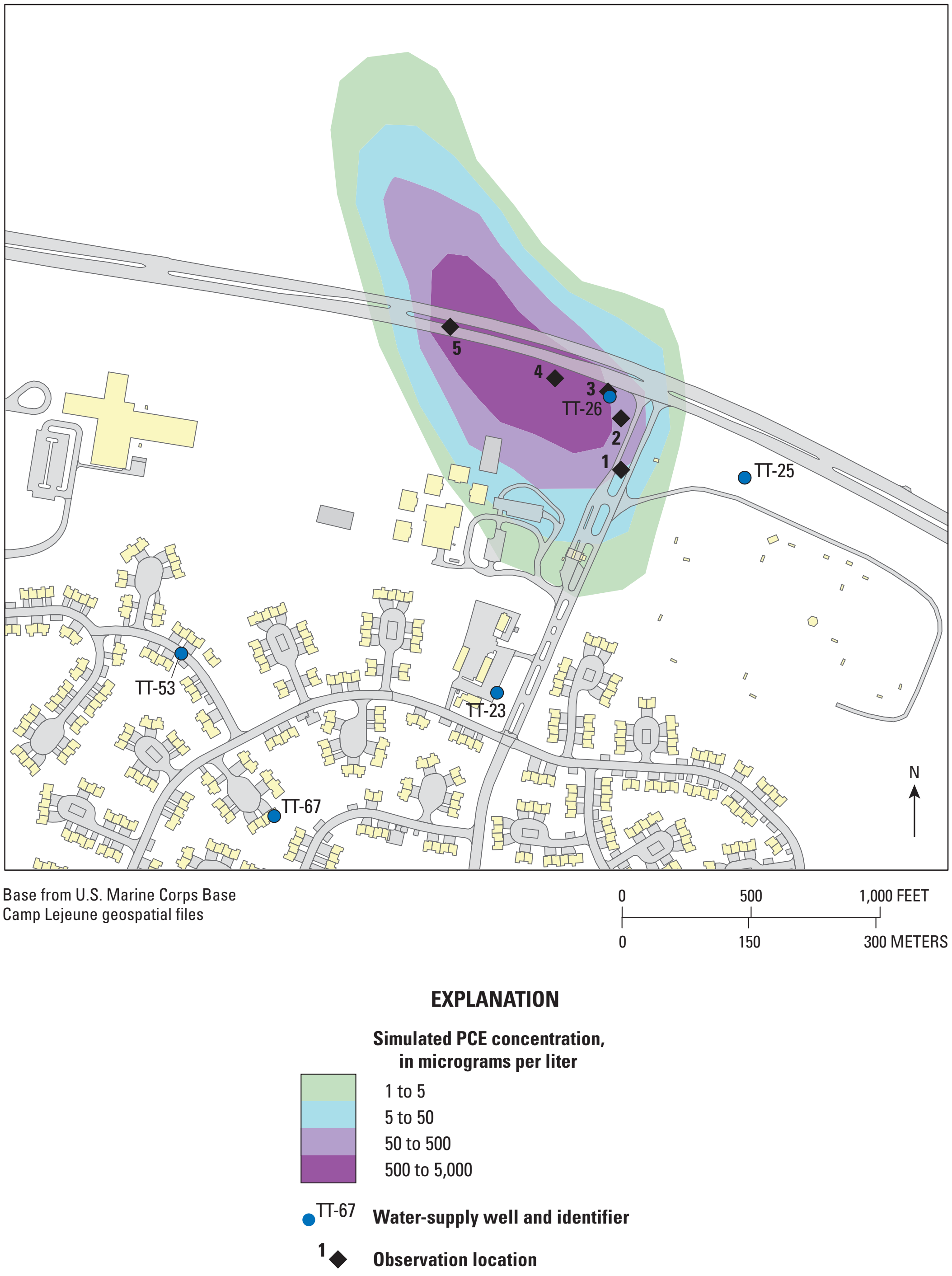
[2] Designation for the model node in the Tarawa Terrace model grid described in Jang and Aral (2008)

[3] Horizontal coordinates referenced to the North American Datum of 1983 (NAD 83)

[4] Observation location 3 corresponds to Tarawa Terrace water-supply well TT-26. Well construction details for TT-26 obtained from Faye and Valenzuela (2007)

---

[4] Modified from the original study described in Jang and Aral (2008) and Wang and Aral (2008).



Base from U.S. Marine Corps Base Camp Lejeune geospatial files

Figure S5.13. Observation locations for Tarawa Terrace simulations, Tarawa Terrace analysis area, U.S. Marine Corps Base Camp Lejeune, North Carolina. [Note: Simulated tetrachloroethylene (PCE) concentrations derived using calibrated Tarawa Terrace numerical model parameters (Jang and Aral 2008); see text for details]

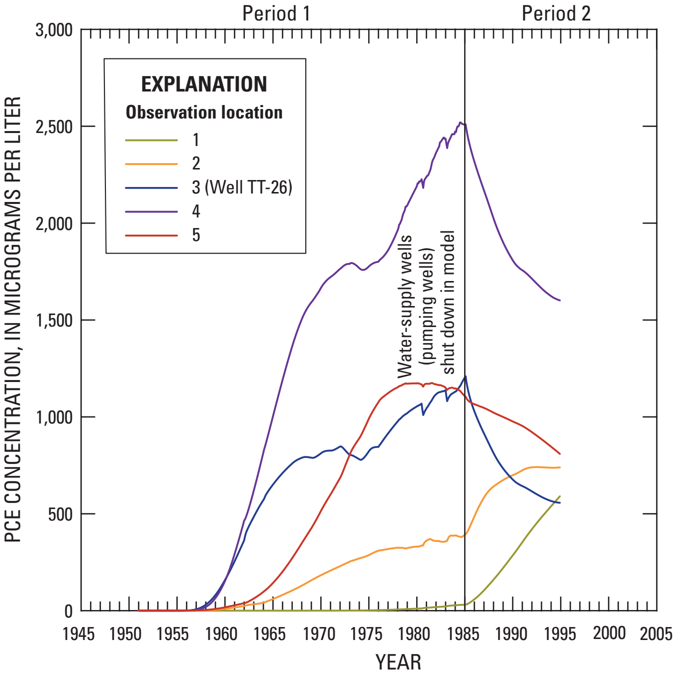


Figure S5.14. Simulated tetrachloroethylene (PCE) concentration versus time at selected Tarawa Terrace observation locations, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.13 for observation locations]

The addition of internal data is also evaluated in the LCM verification task. Recall that internal data are contaminant data that are available at the observation locations during the period in which we are attempting to reconstruct the contaminant history. The internal data in this case are simulated PCE concentrations at selected points in time during Period 1 (January 1951–December 1984) (Table S5.2, Figure S5.15). Three scenarios are explored:

- Internal data are not available (Scenario 1; Figure S5.14)
- Eight internal data points are available (Scenario 2; Figure S5.15*A*)
- Fifteen internal data points are available (Scenario 3; Figure S5.15*B*)

Additional relevant site data include well construction details and information about the subsurface geology and aquifer systems in the Tarawa Terrace analysis area. These data and information are included in a previously published report (Faye and Valenzuela 2007).

Table S5.2. Internal data points selected from the Tarawa Terrace simulation, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[µg/L, microgram per liter; —, not available; TT-26, Tarawa Terrace water-supply well]

Observation location[1]	Tarawa Terrace model node[2]	Date	PCE concentration, in µg/L
Scenario 1: No internal data points			
—	—	—	—
Scenario 2: Eight internal data points			
1	102570	June 1977	0.68
2	103438	October 1971	223.84
2	103438	April 1979	325.63
3, TT-26	103860	August 1967	779.52
4	104066	June 1963	698.08
4	104066	June 1973	1,790.88
5	104892	April 1964	106.79
5	104892	December 1975	1,069.55
Scenario 3: Fifteen internal data points			
1	102570	August 1967	0.051
1	102570	December 1980	14.57
2	103438	October 1971	223.84
2	103438	December 1975	307.90
2	103438	April 1979	325.63
3, TT-26	103860	April 1959	97.29
3, TT-26	103860	August 1967	779.52
3, TT-26	103860	February 1980	1,056.90
4	104066	October 1956	2.03
4	104066	December 1960	278.67
4	104066	June 1973	1,790.88
4	104066	August 1977	1,915.58
5	104892	April 1964	106.79
5	104892	October 1971	663.37
5	104892	August 1977	1,141.87

[1] See Figure S5.13 for observation locations

[2] Designation for the model node in the Tarawa Terrace model grid described in Jang and Aral (2008)

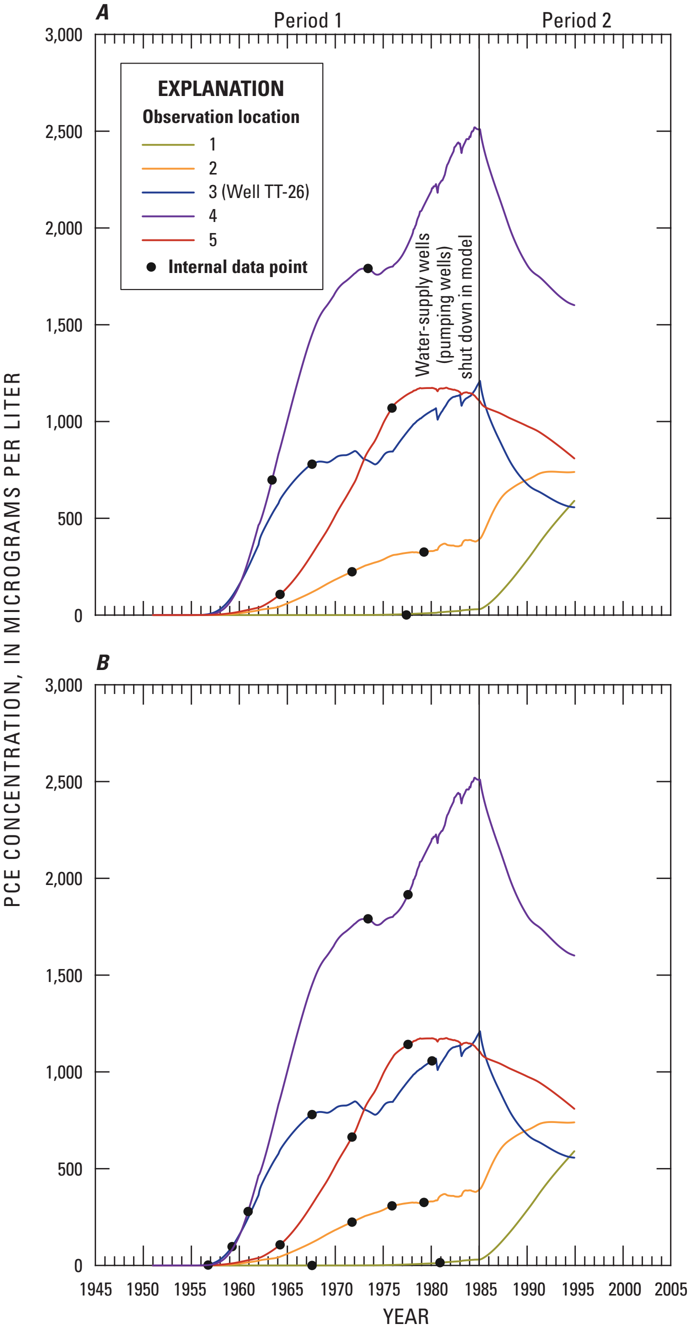


Figure S5.15. Simulated tetrachloroethylene (PCE) versus time and internal data for two Tarawa Terrace analysis scenarios: *(A)* Scenario 2, with 8 internal data points, and *(B)* Scenario 3, with 15 internal data points, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.13 for observation locations]

LCM Application for the HPLF Analysis Area

The objective for the LCM application for the HPLF analysis area is to reconstruct the history of the contaminants at water-supply well HP-651 for the time period before it was shut down in February 1985. The LCM application is focused on characterizing aquifer and contaminant behavior locally around HP-651 (Figures S5.2 and S5.3). Relevant information for applying the LCM approach includes the operational schedule of HP-651, the operational schedule of other water-supply wells and remediation wells in the immediate vicinity of HP-651, and measured contaminant concentrations in groundwater at observation locations around HP-651. Only the forward time integration form of the LCM approach is used for the HPLF application.

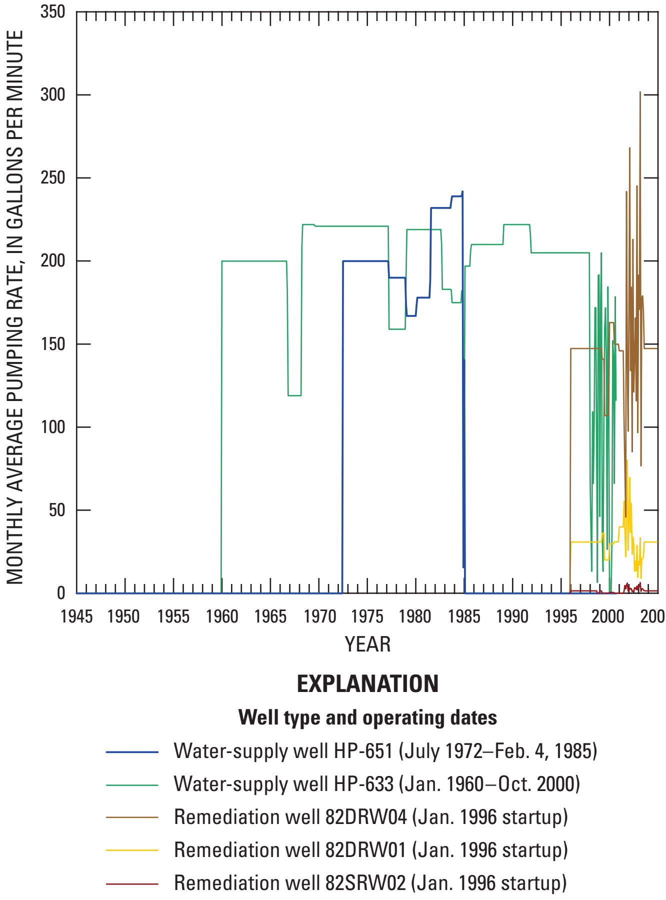


Figure S5.16. Operational schedule for well HP-651, well HP-633, and representative remediation wells in the vicinity of well HP-651, Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.4 for well locations]

The historical operating schedules for water-supply well HP-651, water-supply well HP-633 (the closest downgradient water-supply well), and selected representative remediation wells are illustrated in Figure S5.16. The schedules for the water-supply wells correspond to the maximum monthly average pumping rate and operating times developed in a separate project that focused on characterizing water-supply well operations in the Hadnot Point and Holcomb Boulevard water-supply areas of USMCB Camp Lejeune (Sautner et al. 2013; Telci et al. 2013). The HP-633 schedule is more variable during and after January 1998 because actual operational data were used for that period. The schedules for the remediation wells were developed from monthly operating data provided in historical annual monitoring reports (CH2M HILL, Inc. and Baker Environmental, Inc. 2002; Engineering and Environment, Inc. and Michael Baker Jr., Inc. 2005). Of the 10 remediation wells in the vicinity of HP-651, data from only 3 are shown in Figure S5.16. Typical operation for the shallow remediation wells is represented by 82SRW02, and typical operation for the deep remediation wells is represented by 82DRW01. The operation of 82DRW04 is unique; therefore, data from that well are also shown in Figure S5.16. The mean monthly pumping rate for the shallow wells was less than 2 gallons per minute (gpm), and the mean monthly pumping rate for three of the four deep wells was less than 40 gpm. Remediation well 82DRW04 had a mean monthly pumping rate of 146 gpm. Aside from 82DRW04, the pumping rates for the remediation wells were relatively low compared to the pumping rates of the water-supply wells. To simplify the system, the operation of the remediation wells is excluded from the LCM application.

Prior to 1985, measurements of contaminant concentration in the groundwater surrounding HP-651 are not available. Limited data exist from groundwater sampling events at HP-651 conducted in early 1985, 1986, and 1991. Additional contaminant concentration data are available beginning in 1986, when monitoring wells were installed to characterize the nature and extent of groundwater contamination in the area. A summary of reported analytical results for PCE, TCE, and associated degradation products for all of the water-supply wells, monitor wells, and remediation wells in the HPLF analysis area is included in a previous ATSDR data report (Faye et al. 2010). Because the LCM application is focused on characterizing aquifer behavior locally around HP-651, contaminant data for selected wells in the HPLF analysis area that are within 1,000 ft of HP-651 were evaluated for use in this analysis (Table S5.3 [at back of report], Figure S5.4).

Additional site data that are relevant to the reconstruction problem include well construction details and information about the subsurface geology and aquifer systems in the HPLF. These data are included in previously published reports (Faye et al. 2010; Faye 2012).

Results

PCE is the contaminant of interest in the Tarawa Terrace analysis area. Results of the LCM verification using synthetic data from the previously developed Tarawa Terrace numerical model are presented for the forward and backward time integration procedures.

For the HPLF application, PCE, TCE, 1,2-tDCE, and VC are included in the LCM reconstruction. Given the similarity in results at Tarawa Terrace between the forward and backward time integration forms of the LCM approach, only the forward time integration method is used for the HPLF application.

LCM Verification at Tarawa Terrace

For the Tarawa Terrace analysis area, the forward and backward time integration procedures of the LCM approach use the same time periods for analysis:

- Period 1 extends from January 1951 through December 1984, and
- Period 2 extends from December 1984 through December 1994.

LCM Results Using Forward Time Integration

LCM results obtained by using the forward time integration procedure to reconstruct PCE concentrations at five selected observation locations are shown in Figure S5.17. The Tarawa Terrace numerical simulation results, which in this case represent the expected or known values, are included for comparison. The LCM results at the end of Period 1 (beginning of Period 2) are very close to the expected results from the numerical simulation. This indicates that the conditions set up in the optimization model are satisfied. Concentrations were successfully reconstructed during Period 1 for all five observation locations.

At observation locations 3 and 4, the LCM method without internal data points overestimates the magnitude of the maximum concentration, and the timing of the peak concentration occurs earlier than expected (Figure S5.17*B*). The overestimation and temporal offset are both remedied as more internal data are included in the method (Figures S5.17*C* and S5.17*D*).

At observation locations 3, 4, and 5, the first appearance (arrival) of the reconstructed concentrations occurs earlier in time than expected. This is attributed to the dependence of the reconstructed concentrations on the initial water-supply well pumping rates at the first time step (Equation S5.15). The initial pumping rates are non-zero in this analysis, which generates an earlier than expected concentration for several of the observation locations. If the initial pumping rates were zero, the reconstructed concentrations would be later than expected. The effect of initial pumping rates may diminish as time progresses. The backward time integration procedure reduces this effect.

Coefficients of the system matrices $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{B}}$ that are associated with these LCM results are listed in Tables S5.4 and S5.5, respectively. Recall that the coefficients of matrix $\widehat{\mathbf{A}}$ represent the characteristics or behavior of the aquifer system during Period 2 and the coefficients of matrix $\widehat{\mathbf{B}}$ represent the behavior of the groundwater system during Period 1.

The diagonal elements of the matrix $\widehat{\mathbf{A}}$ have a value close to one, implying that the concentration at any given observation location and time step depends primarily on the concentration at that location for the previous time step. Contaminant concentrations at other observation locations have some minor effect, as indicated by the non-zero values of the off-diagonal coefficients.

The coefficients of matrix $\widehat{\mathbf{B}}$ in this case are relatively large because the water-supply well pumping rate values are in units of cubic meters per second. Water-supply well TT-26 is the closest pumping well to the contaminant source; therefore, well TT-26 has a significant influence on the contaminant concentration distribution (Figure S5.13). Water-supply wells TT-67 and TT-53 are further away from the contaminant source, but they may have some influence on the contaminant distribution. Because the groundwater flow direction in the absence of pumping is expected to be southward, toward Northeast Creek, the southward influence contributed from water-supply wells TT-67 and TT-53 is difficult to discern. The magnitudes of the coefficients of matrix $\widehat{\mathbf{B}}$ are in general agreement with the expected physical behavior of the groundwater system.

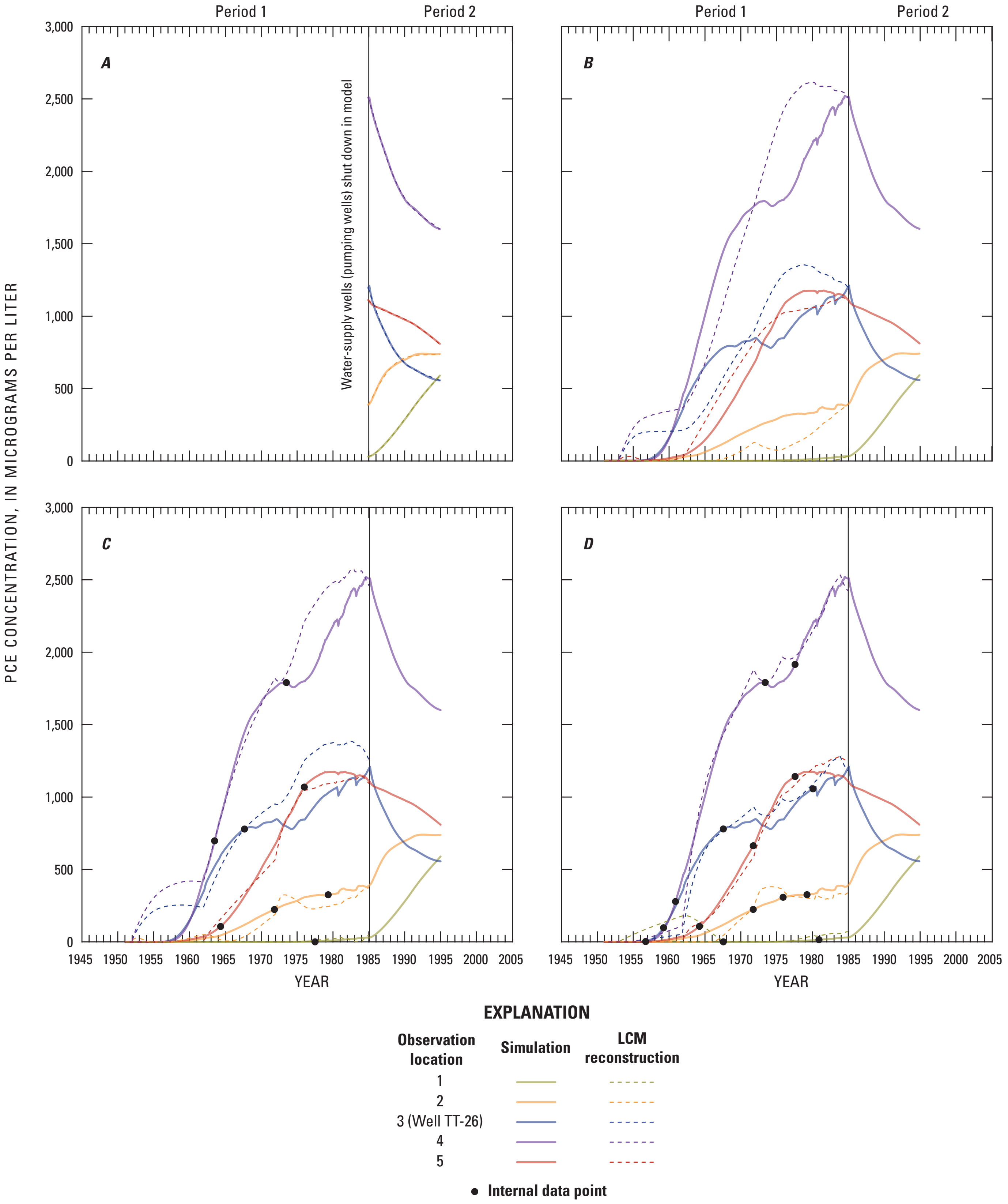


Figure S5.17. Linear control model (LCM) results using the forward time integration procedure to reconstruct tetrachloroethylene (PCE) concentration during *(A)* Period 2, *(B)* Period 1 with no internal data, *(C)* Period 1 with 8 internal data points, and *(D)* Period 1 with 15 internal data points, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.13 for observation locations]

Table S5.4. Coefficients of the system matrix $\hat{\mathbf{A}}$ identified using the method of least squares, Tarawa Terrace analysis area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[TT-26, Tarawa Terrace water-supply well]

Observation location[1]	1 (node 102570)	2 (node 103438)	3 Water-supply well TT-26 (node 103860)	4 (node 104066)	5 (node 104892)
1 (node 102570)	0.997416	−0.005763	−0.033919	0.014210	0.007749
2 (node 103438)	0.004879	0.901272	−0.197240	0.110160	0.004020
3, TT-26 (node 103860)	0.020670	−0.029186	0.983513	−0.015668	0.051779
4 (node 104066)	0.032446	−0.036412	0.010031	0.963687	0.071000
5 (node 104892)	−0.002807	−0.043846	−0.104890	0.052159	1.006345

[1] See Figure S5.13 for observation locations. Node numbers refer to the model node in the Tarawa Terrace model grid described in Jang and Aral (2008)

Table S5.5. Coefficients of the system matrix $\hat{\mathbf{B}}$ for the forward time integration procedure, Tarawa Terrace analysis area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Observation location[1]	Water-supply well TT-26	Water-supply well TT-53	Water-supply well TT-67
1 (node 102570)	−166.11	−215.12	351.63
2 (node 103438)	−126.35	−580.85	−598.83
3, TT-26 (node 103860)	919.64	470.74	784.69
4 (node 104066)	1,164.19	902.85	433.82
5 (node 104892)	416.77	762.66	255.98

[1] See Figure S5.13 for observation locations. Node numbers refer to the model node in the Tarawa Terrace model grid described in Jang and Aral (2008)

LCM Results using Backward Time Integration

LCM results obtained by using the backward time integration procedure to reconstruct PCE concentrations at the same five selected observation locations are shown in Figure S5.18. Again, the Tarawa Terrace numerical simulation results, which represent the accepted or known values, are included for comparison.

The backward time integration procedure reduces the effect that the initial water-supply well pumping rates have on the reconstructed concentrations. In the case of the forward time integration procedure (Figure S5.17*B*), reconstructed concentrations typically appear earlier in time than expected because they depend on the initial pumping rates in the first time step, which are non-zero in this analysis. The backward time integration procedure provides a better estimate of the timing of contaminant breakthrough at a given observation location (Figure S5.18*B*); this estimate is independent of the initial status (pumping/not pumping) of the water-supply wells.

Error Analysis

Absolute error and relative error were calculated by comparing the LCM results to the corresponding Tarawa Terrace simulation for each analysis (Tables S5.6 and S5.7; Figure S5.19). The Tarawa Terrace simulation represents the expected or known values for evaluation purposes. The absolute error is calculated by

$$e_i = \frac{1}{N}\sum_{k=1}^{N}\left|x_i(k) - x_i^*(k)\right| , \qquad \text{(S5.37)}$$

and the relative average error is calculated by

$$re_i(\%) = \frac{100e_i}{\frac{1}{N}\sum_{k=1}^{N} x_i^*(k)} , \qquad \text{(S5.38)}$$

where N is the number of monthly stress periods used in the model simulation.

Observation locations with relatively lower concentrations (i.e., observation locations 1 and 2) have the largest relative error. Overall, the forward time integration procedure has a lower relative average error for most of the observation locations.

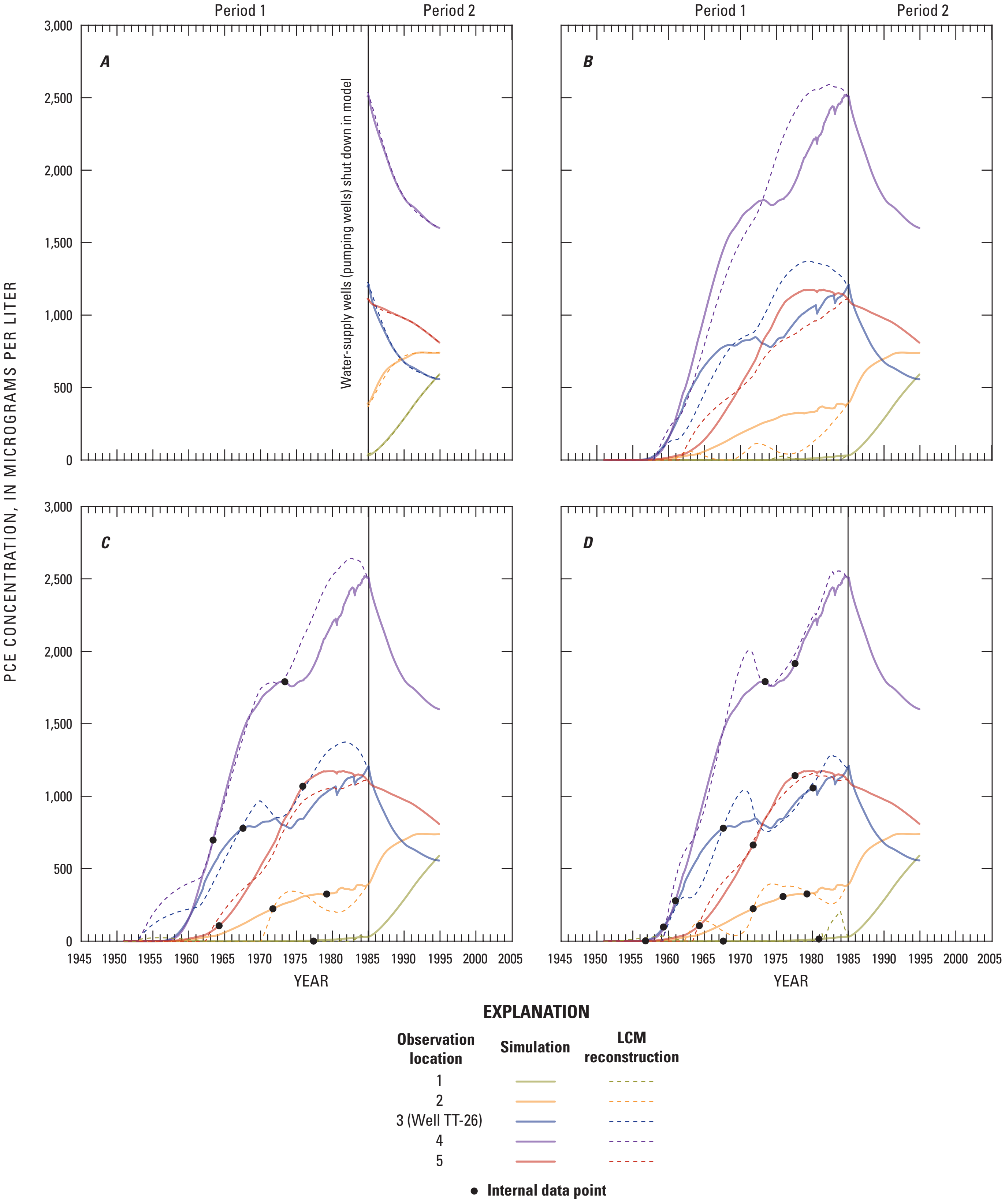


Figure S5.18. Linear control model (LCM) results using the backward time integration procedure to reconstruct tetrachloroethylene (PCE) concentration during *(A)* Period 2, *(B)* Period 1 with no internal data, *(C)* Period 1 with 8 internal data points, and *(D)* Period 1 with 15 internal data points, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.13 for observation locations]

Table S5.6. Error analysis for linear control model results during Period 2, Tarawa Terrace analysis area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[µg/L, microgram per liter; %, percent; TT-26, Tarawa Terrace water-supply well]

Observation location[1]	Average absolute error (µg/L)		Relative average error (%)	
	Forward time integration	Backward time integration	Forward time integration	Backward time integration
1 (node 102570)	1.43	2.93	0.49	1.01
2 (node 103438)	6.71	12.00	1.02	1.83
3, TT-26 (node 103860)	4.51	11.97	0.60	1.59
4 (node 104066)	6.31	14.79	0.33	0.77
5 (node 104892)	2.10	3.60	0.22	0.37

[1] See Figure S5.13 for observation locations. Node numbers refer to the model node in the Tarawa Terrace model grid described in Jang and Aral (2008)

Table S5.7. Error analysis for linear control model results during Period 1, Tarawa Terrace analysis area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[µg/L, micrograms per liter; %, percent; TT-26, Tarawa Terrace water-supply well]

Observation location[1]	Average absolute error (µg/L)			Relative average error (%)		
	Scenario 1 (no internal data)	Scenario 2 (8 internal points)	Scenario 3 (15 internal points)	Scenario 1 (no internal data)	Scenario 2 (8 internal points)	Scenario 3 (15 internal points)
Forward time integration procedure, Period 1						
1 (node 102570)	3.02	2.64	49.66	77.24	67.55	1,272.04
2 (node 103438)	79.55	25.7	35.21	50.78	16.41	22.48
3, TT-26 (node 103860)	187.84	148.72	61.35	31.51	24.95	10.29
4 (node 104066)	261.6	170.51	50.02	22.22	14.48	4.25
5 (node 104892)	71.43	24.25	34.72	14.35	4.87	6.97
Backward time integration procedure, Period 1						
1 (node 102570)	4.37	3.63	15.93	111.96	93.02	408.12
2 (node 103438)	96.79	71.66	48.08	61.78	45.74	30.69
3, TT-26 (node 103860)	144.6	103.52	71.04	24.26	17.37	11.92
4 (node 104066)	161.44	141.72	66.24	13.71	12.04	5.63
5 (node 104892)	93.14	27.14	30.27	18.7	5.45	6.08

[1] See Figure S5.13 for observation locations. Node numbers refer to the model node in the Tarawa Terrace model grid described in Jang and Aral (2008)

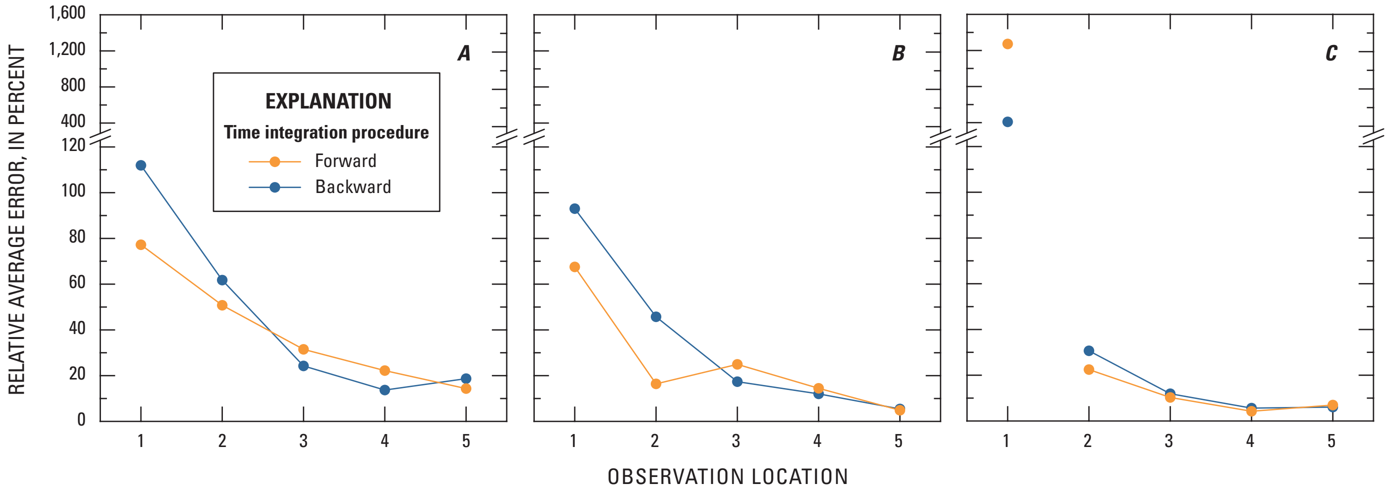


Figure S5.19. Comparison of the relative average error for linear control model (LCM) results for Period 1, scenarios involving *(A)* no internal data, *(B)* 8 internal data points, and *(C)* 15 internal data points, U.S. Marine Corps Base Camp Lejeune, North Carolina.

Uncertainty Analysis

As previously noted, in order to apply the Kalman filter algorithm in the uncertainty analysis, the system noise, measurement error, and certain measurements of contaminant concentration must be determined. The variance of the system noise is calculated based on the field data (measured concentration data), reconstructed concentration data, and the spatial correlation coefficient estimated using the Gaussian spatial correlation model. The measurement error associated with groundwater-quality measurements (i.e., contaminant concentrations) is assumed to have a mean of zero and a variance of 0.1. The measurements of contaminant concentration are calculated using Equation S5.32, where β_i is the average value of the contaminant concentrations generated using LCM and Monte Carlo methods at each observation location for each monthly time step.

For the uncertainty analysis, the LCM reconstruction using the forward time integration procedure and eight internal data points (Scenario 2) is used for illustration. The Monte Carlo simulation is run for 10,000 realizations at each monthly time step. The resulting maximum and minimum contaminant concentration bounds for observation location 3 are shown in Figure S5.20. The confidence intervals corresponding to a confidence level of 80% (10th–90th percentile range of Monte Carlo realizations) are also shown in Figure S5.20. Similarly, the maximum and minimum bounds and confidence intervals are shown for observation locations 4 and 5 in Figures S5.21 and S5.22, respectively.

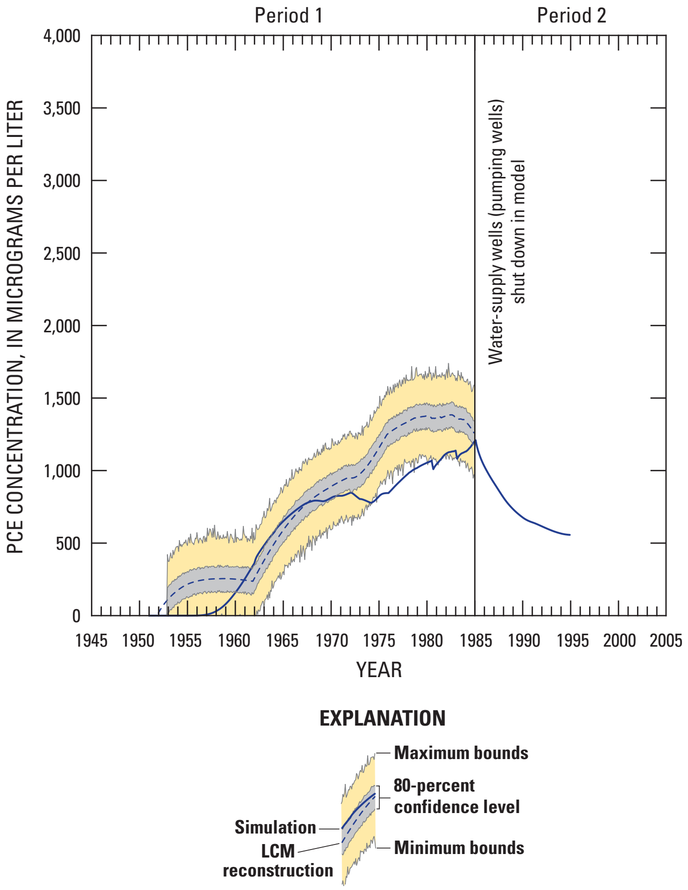


Figure S5.20. Monte Carlo simulation results for maximum and minimum bounds and 80-percent confidence interval (10–90 percentile range) for tetrachloroethylene (PCE) at observation location 3 (well TT-26), U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.13 for observation location]

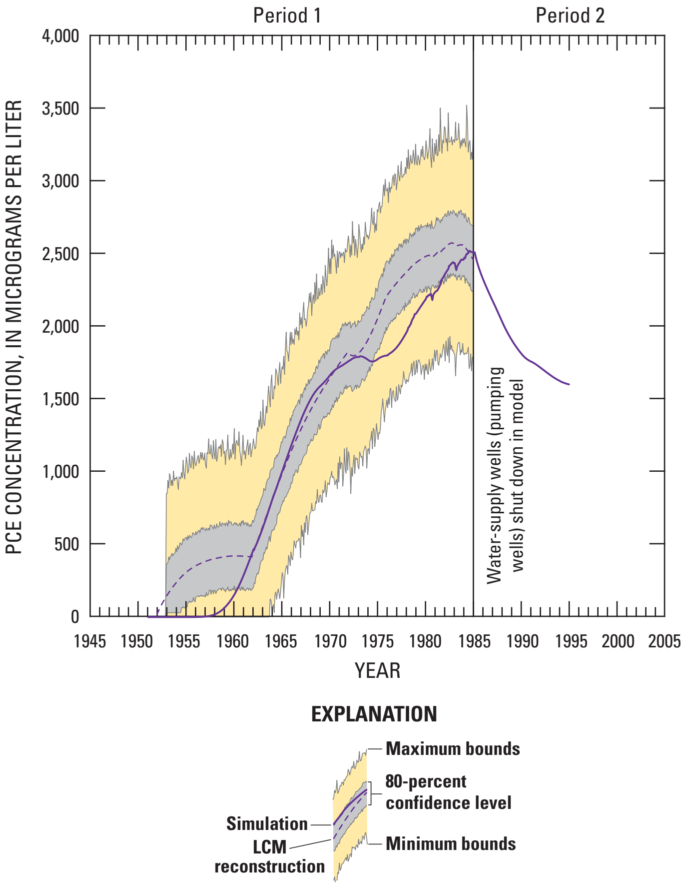


Figure S5.21. Monte Carlo simulation results for maximum and minimum bounds and 80-percent confidence interval (10–90 percentile range) for tetrachloroethylene (PCE) at observation location 4, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.13 for observation location]

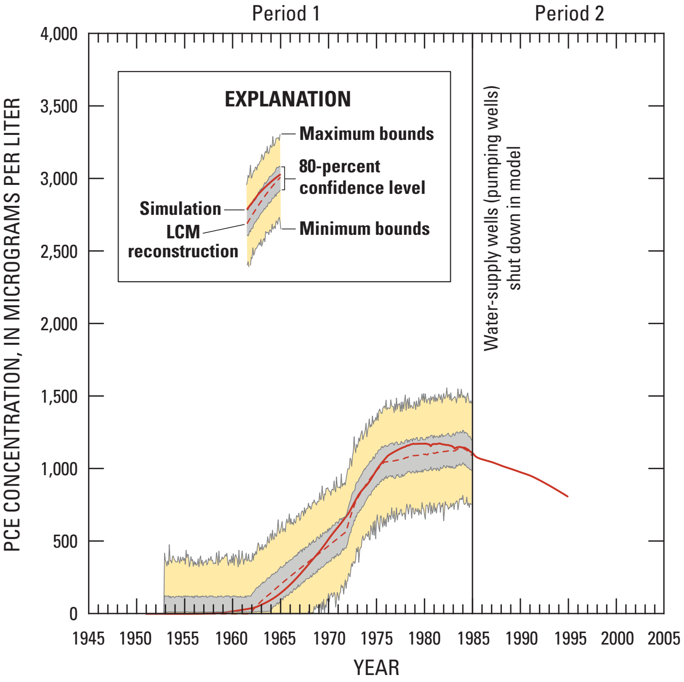


Figure S5.22. Monte Carlo simulation results for maximum and minimum bounds and 80-percent confidence interval (10–90 percentile range) for tetrachloroethylene (PCE) at observation location 5, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.13 for observation location]

LCM Application at the HPLF Analysis Area

Five observation locations were selected for use in the LCM approach based on the availability and quality of contaminant concentration versus time data for wells in close proximity to HP-651 (Table S5.8, Figure S5.23). The contaminant with the highest measured concentration in the HPLF analysis area is TCE. The estimated distribution of TCE in groundwater for pre-remediation conditions (1985–1995) within the Upper Castle Hayne aquifer is shown in Figure S5.23. The historical reconstruction at the five selected observation locations is focused on TCE, PCE, and their associated degradation products 1,2-tDCE and VC. Although 1,1-dichloroethylene (1,1-DCE) and *cis*-1,2-dichloroethylene (1,2-*c*DCE) are also degradation products that are often of interest, the measured data for these contaminants are not adequate for inclusion in the LCM reconstruction. Given the similarity in results for Tarawa Terrace between the forward and backward time integration forms of the LCM approach, only the forward time integration method is used for the HPLF application.

Final deterministic LCM results obtained using the forward time integration procedure to reconstruct PCE, TCE, 1,2-tDCE, and VC concentrations at water-supply well HP-651 are shown in Figure S5.24. Results for each contaminant are presented on the same logarithmic scale to facilitate visual comparison. Selected interim results from the LCM process as well as the stochastic results from uncertainty analyses are presented for PCE, TCE, 1,2-tDCE, and VC in the following subsections.

Table S5.8. Observation locations for the Hadnot Point landfill (HPLF) analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[NC SPCS, North Carolina State Plane Coordinate System; PCE, tetrachloroethylene; TCE, trichloroethylene; 1,2-tDCE, *trans*-1,2-dichloroethylene; VC, vinyl chloride]

Observation location[1]	Easting coordinate, in feet NC SPCS[2]	Northing coordinate, in feet NC SPCS[2]	Well screen altitude, in feet[3]	Contaminants
HP-651	2503829	348083	−93 to −103 −108 to −123 −157 to −162	PCE, TCE, 1,2-tDCE, VC
06-GW34	2503483	348434	9.7 to −5.6	PCE, TCE, 1,2-tDCE
82-SRW02	2503512	348700	−8 to −28	VC
82-DRW01	2503431	348098	−47.8 to −67.8	PCE, TCE, 1,2-tDCE, VC
82-DRW04	2503128	348391	−68.4 to −88.4	PCE, TCE, 1,2-tDCE, VC

[1] See Figure S5.23 for observation locations. Coordinates and well-screen information for the listed observation locations were obtained from Faye et al. (2010)

[2] Horizontal coordinates referenced to the North American Datum of 1983 (NAD 83)

[3] Referenced to the National Geodetic Vertical Datum of 1929 (NGVD 29)

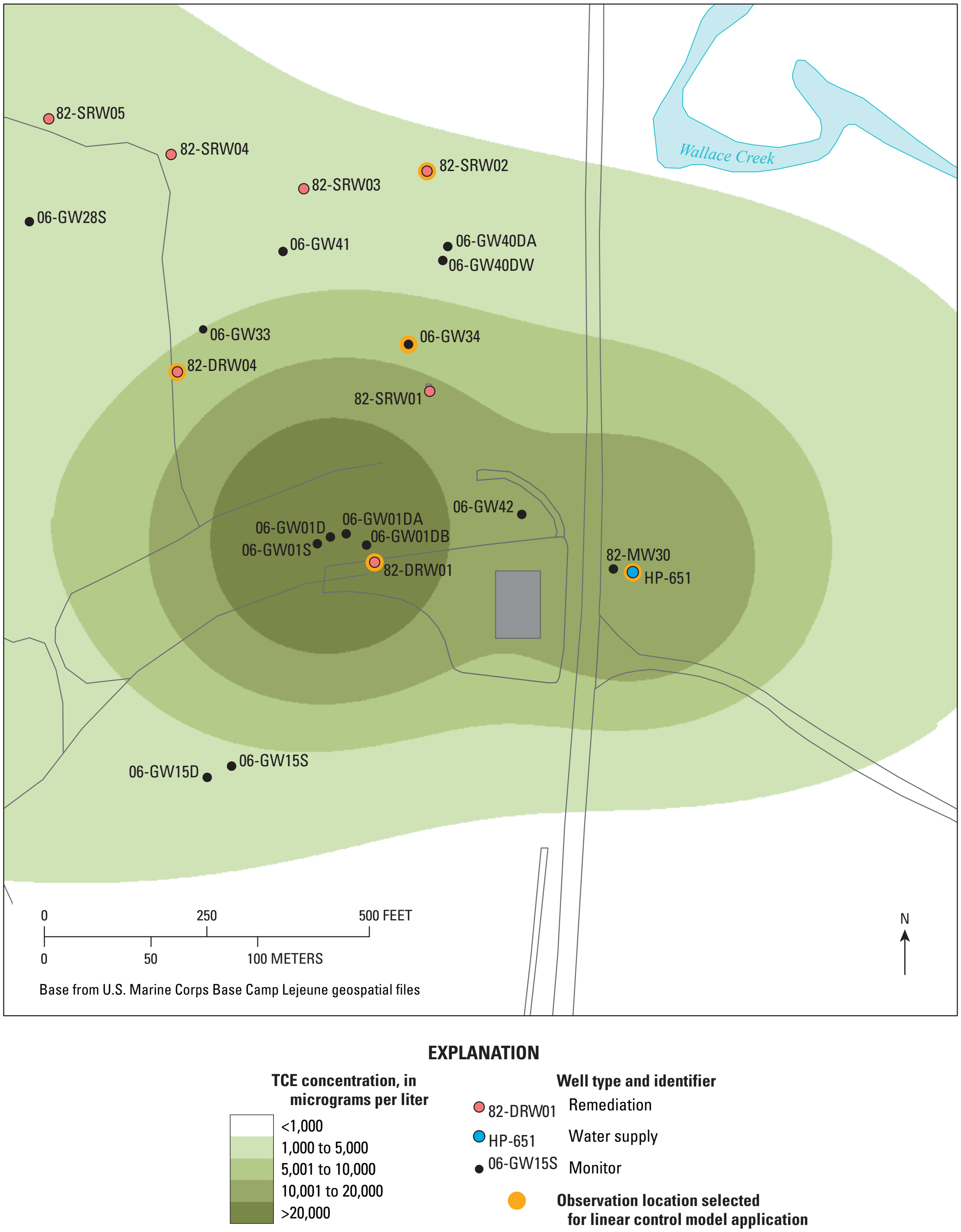


Figure S5.23. Selected observation locations for linear control model application, Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

LCM Results for Tetrachloroethylene (PCE)

Before obtaining the final results for the reconstruction of PCE at water-supply well HP-651 that are presented in Figure S5.24*A*, several interim results or determinations are developed as part of the LCM process. These interim, stepwise determinations include

- The designation of model time periods for the PCE reconstruction as January 1943–January 1992 (Period 1) and January 1992–July 2004 (Period 2). This designation is made in part by the availability of measured contaminant data at the selected observation locations.
- The results of fitting a continuous mathematical function to the discrete measured concentration versus time data at each selected observation location (Figure S5.25). Results from the fitted models during Period 2 (January 1992–July 2004) are used collectively to identify the coefficients of system matrix $\widehat{\mathbf{A}}$ as previously described.
- Two internal data points for water-supply well HP-651 selected for use in the LCM optimization during Period 1 (Table S5.9).

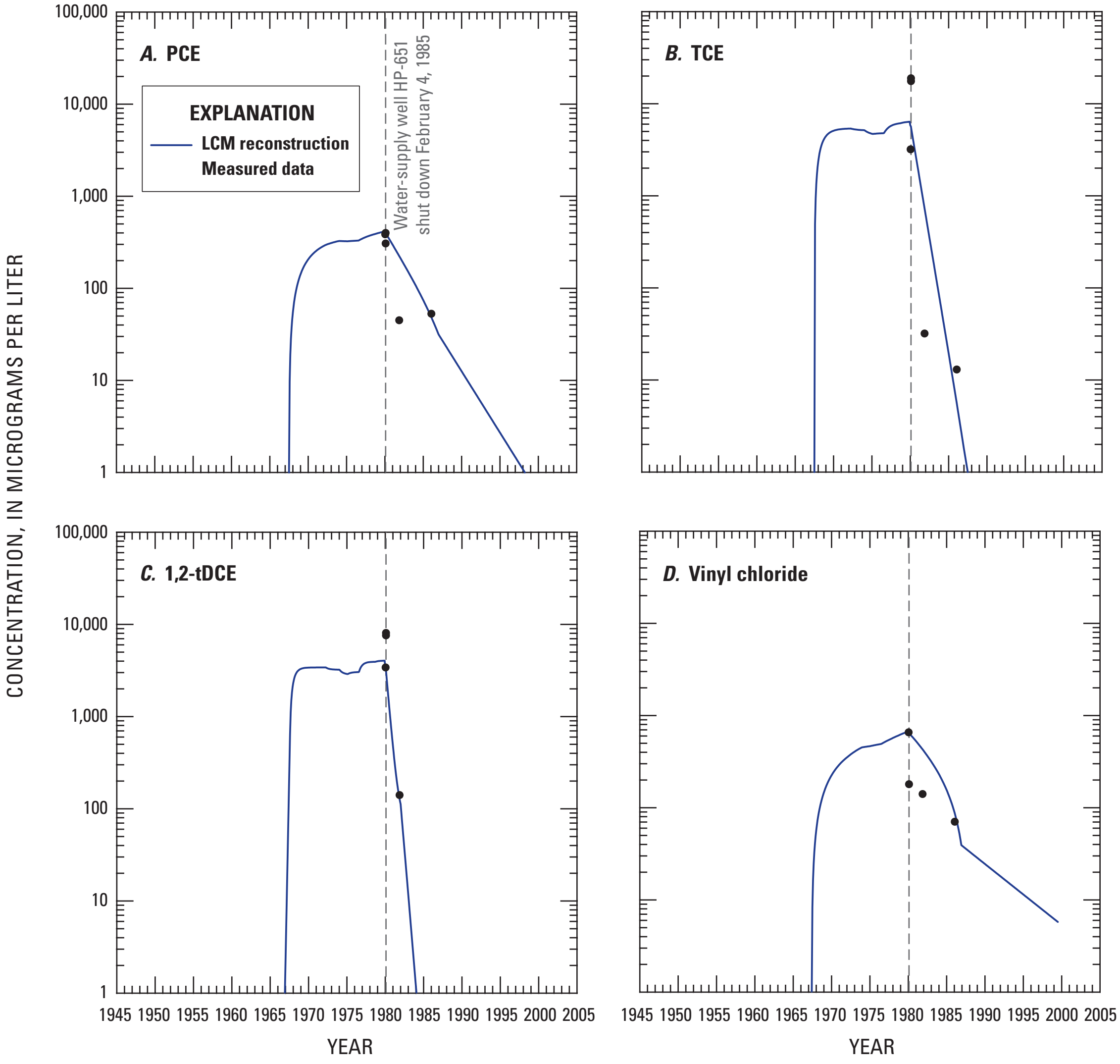


Figure S5.24. Deterministic results using the linear control model to reconstruct contaminant concentrations over time at water-supply well HP-651 for *(A)* tetrachloroethylene (PCE), *(B)* trichloroethylene (TCE), *(C)* 1,2-*trans*-dichloroethylene (1,2-tDCE), and *(D)* vinyl chloride (VC), U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well location]

- Coefficients of the system matrices $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{B}}$ that are associated with the final LCM results (Tables S5.10 and S5.11, respectively). The coefficients of matrix $\widehat{\mathbf{A}}$ represent the characteristics or behavior of the groundwater aquifer system during Period 2, and the coefficients of matrix $\widehat{\mathbf{B}}$ represent the behavior of the groundwater system during Period 1.

Table S5.9. Internal data points for PCE selected for use in linear control model optimization during Period 2 (1992–2004), U.S. Marine Corps Base Camp Lejeune, North Carolina.

[PCE, tetrachloroethylene; µg/L, microgram per liter]

Observation location[1]	Date	PCE concentration, in µg/L
HP-651	2/04/1985	400
HP-651	1/22/1991	53

[1] See Figure S5.23 for well location

Table S5.10. Coefficients of the system matrix $\hat{\mathbf{A}}$ identified using PCE data during Period 2 (1992–2004), U.S. Marine Corps Base Camp Lejeune, North Carolina.

[PCE, tetrachloroethylene]

Observation location[1]	Monitor well 06-GW34	Remediation well 82-DRW01	Remediation well 82-DRW04	Water-supply well HP-651
06-GW34	1.01869	−0.00002	0.00054	0.00082
82-DRW01	0	0.99513	0	0.00043
82-DRW04	−0.00001	0	1.01248	0.00007
HP-651	0	0	0	0.97479

[1] See Figure S5.23 for well locations

Table S5.11. Coefficients of the system matrix $\hat{\mathbf{B}}$ identified using linear control model optimization procedure with two internal data points for PCE, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[PCE, tetrachloroethylene]

Observation location[1]	Water-supply well HP-651	Water-supply well HP-633
06-GW34	0.00494	−0.00537
82-DRW01	0.04813	0.05351
82-DRW04	0.03202	−0.02711
HP-651	0.05093	−0.00218

[1] See Figure S5.23 for well locations

- Deterministic LCM results obtained by using the forward time integration procedure to reconstruct PCE concentrations at HP-651 and selected adjacent observation locations (Figure S5.26).
- Stochastic results for the uncertainty analysis conducted during Period 1 using 10,000 Monte Carlo realizations at each monthly time step. The resulting maximum and minimum contaminant concentration bounds for water-supply well HP-651 are shown in Figure S5.27. The confidence intervals corresponding to a confidence level of 95% (representing the 2.5–97.5 percentile range of Monte Carlo realizations) also are shown in Figure S5.27.

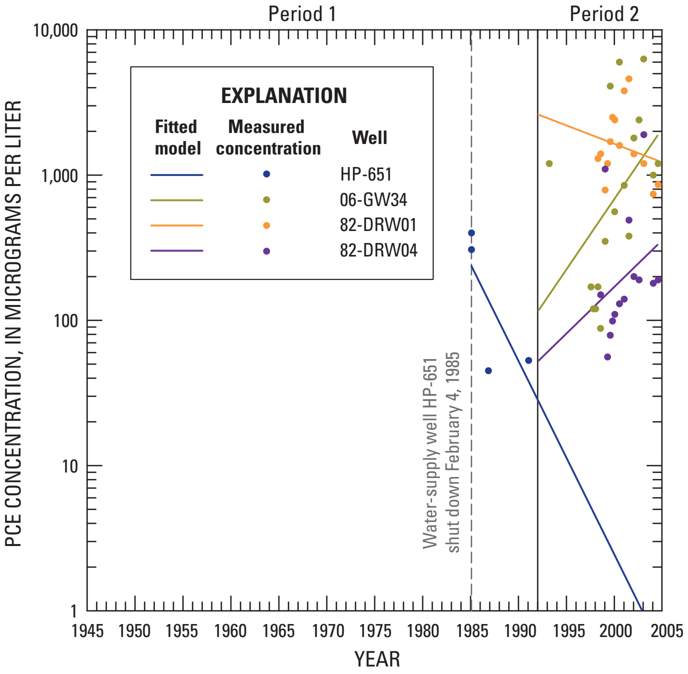


Figure S5.25. Measured tetrachloroethylene (PCE) concentration data over time and fitted model of the data for selected Hadnot Point landfill locations, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well locations]

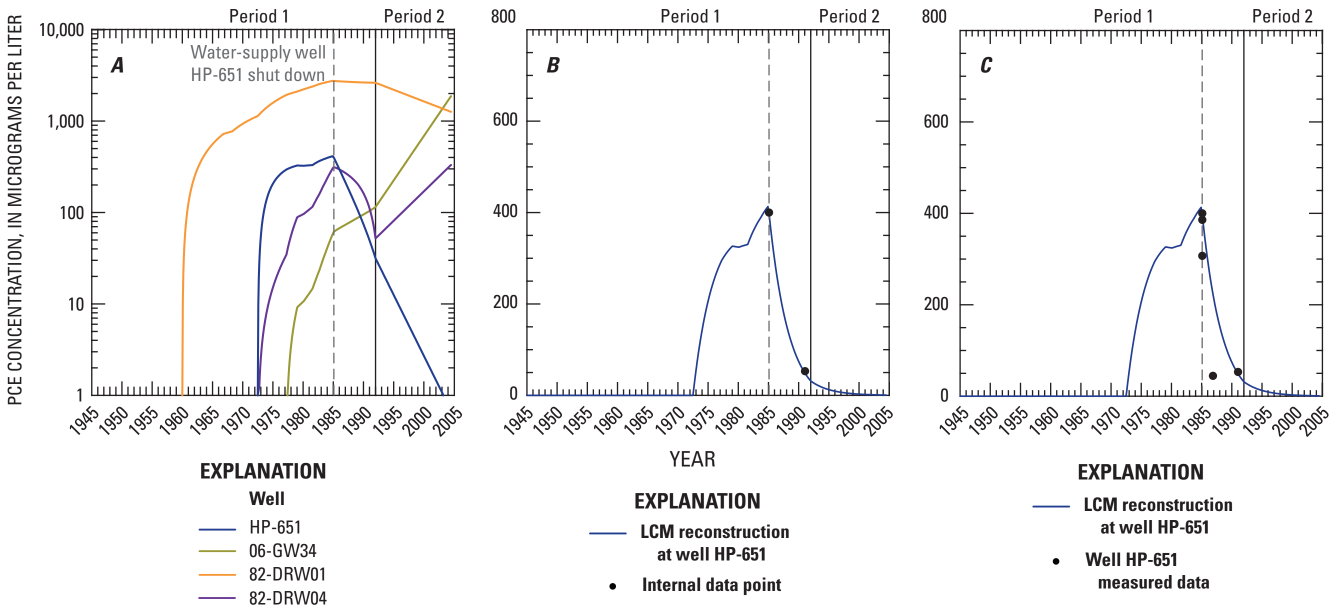


Figure S5.26. Linear control model results for reconstruction of tetrachloroethylene (PCE) concentration over time *(A)* at four selected locations, *(B)* at HP-651, with two internal data points used in the analysis, and *(C)* at HP-651 with measured PCE data, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well locations]

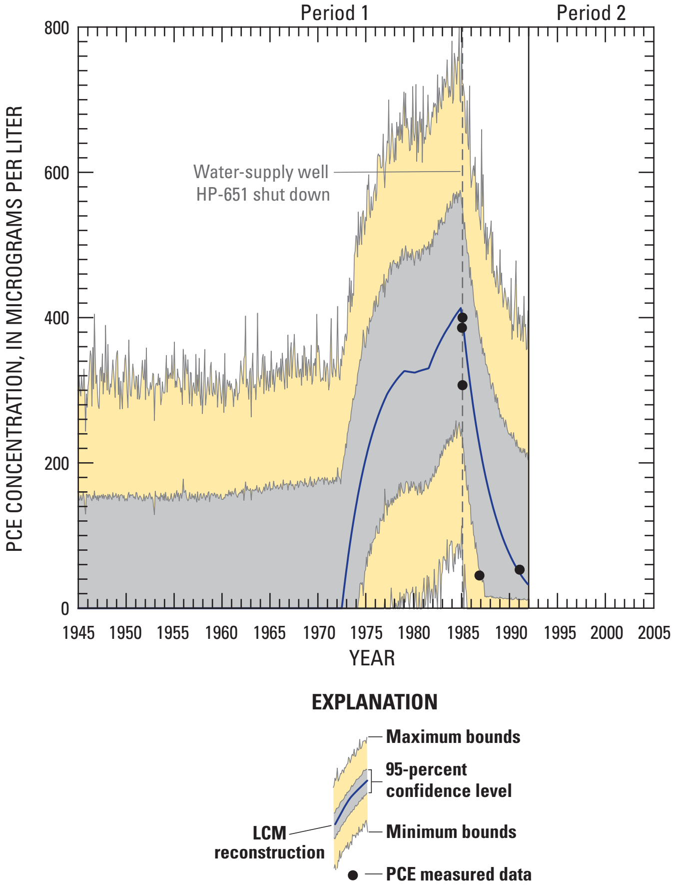


Figure S5.27. Monte Carlo simulation results for maximum and minimum bounds and 95-percent confidence interval (2.5–97.5 percentile range) for tetrachloroethylene (PCE) concentration reconstructed at water-supply well HP-651, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well location]

LCM Results for Trichloroethylene (TCE)

The final deterministic results for the reconstruction of TCE at water-supply well HP-651 are presented in Figure S5.24*B*. The interim, step-wise determinations developed during the LCM process include

- The definition of model time periods for the TCE reconstruction as January 1943–January 1992 (Period 1) and January 1992–July 2004 (Period 2).
- The results of fitting a continuous mathematical function to the discrete measured TCE concentration versus time data at each selected observation location (Figure S5.28). Results from the fitted models during Period 2 (January 1992–July 2004) are used collectively to identify the coefficients of system matrix $\widehat{\mathbf{A}}$.
- Seven internal data points at water-supply well HP-651 selected for use in the LCM optimization during Period 1 (Table S5.12).
- Coefficients of the system matrices $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{B}}$ that are associated with the final LCM results (Tables S5.13 and S5.14, respectively).
- Deterministic LCM results obtained by using the forward time integration procedure to reconstruct TCE concentrations at HP-651 and selected adjacent observation locations (Figure S5.29).
- Stochastic results for the uncertainty analysis conducted during Period 1 using 10,000 Monte Carlo realizations at each monthly time step. The resulting maximum and minimum contaminant concentration bounds for water-supply well HP-651 are shown in Figure S5.30. The confidence intervals corresponding to a confidence level of 95% (representing the 2.5–97.5 percentile range of Monte Carlo results) also are shown in Figure S5.30.

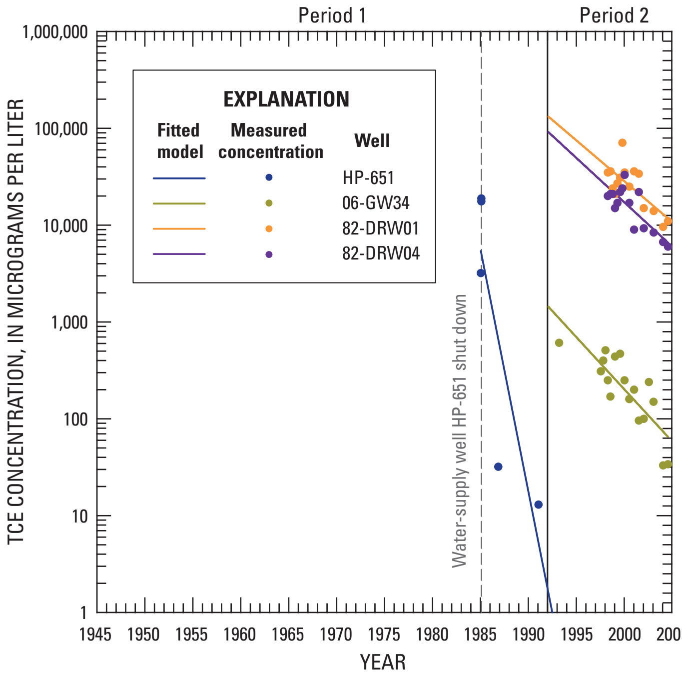


Figure S5.28. Measured trichloroethylene (TCE) concentration data over time and fitted model of the data for selected Hadnot Point landfill locations, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well locations]

Table S5.12. Internal data points for TCE selected for use in linear control mode optimization during Period 2 (1992–2004), U.S. Marine Corps Base Camp Lejeune, North Carolina.

[TCE, trichloroethylene; µg/L, microgram per liter]

Observation location[1]	Date	TCE concentration, in µg/L
HP-651	2/1/1985	5,138
HP-651	2/1/1986	1,790
HP-651	2/1/1987	565.5
HP-651	2/1/1988	178.6
HP-651	2/1/1989	56.2
HP-651	2/1/1990	17.8
HP-651	2/1/1991	5.6

[1] See Figure S5.23 for well location

Table S5.13. Coefficients of the system matrix $\hat{\mathbf{A}}$ identified using TCE data during Period 2 (1992–2004), U.S. Marine Corps Base Camp Lejeune, North Carolina.

[TCE, trichloroethylene]

Observation location[1]	Monitor well 06-GW34	Remediation well 82-DRW01	Remediation well 82-DRW04	Water-supply well HP-651
06-GW34	0.97891	−0.00001	0.00003	0.030010
82-DRW01	−0.03468	0.98337	0.00140	1.90091
82-DRW04	−0.02984	−0.00052	0.98380	1.52188
HP-651	−0.00001	0	0	0.90996

[1] See Figure S5.23 for well locations

Table S5.14. Coefficients of the system matrix $\hat{\mathbf{B}}$ identified using linear control model optimization procedure with seven internal data points for TCE, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[TCE, trichloroethylene]

Observation location[1]	Water-supply well HP-651	
06-GW34	1.39370	−0.26017
82-DRW01	−7.87872	−1.77102
82-DRW04	−4.70253	−1.48884
HP-651	2.46493	−0.00007

[1] See Figure S5.23 for well locations

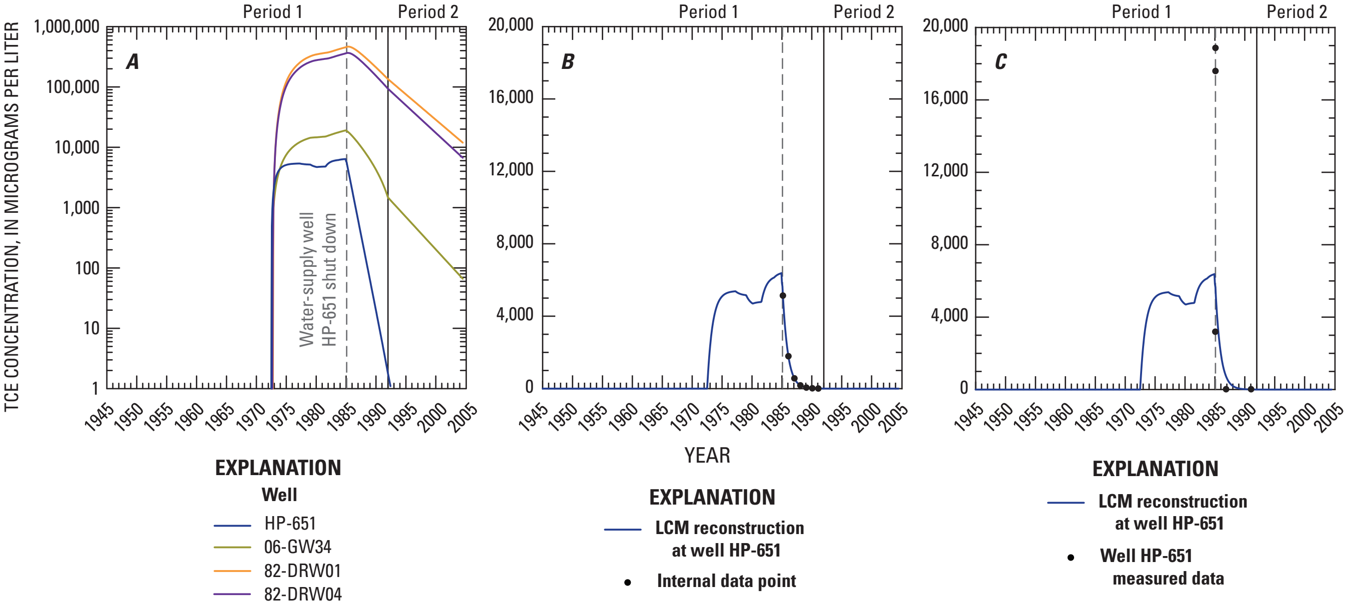
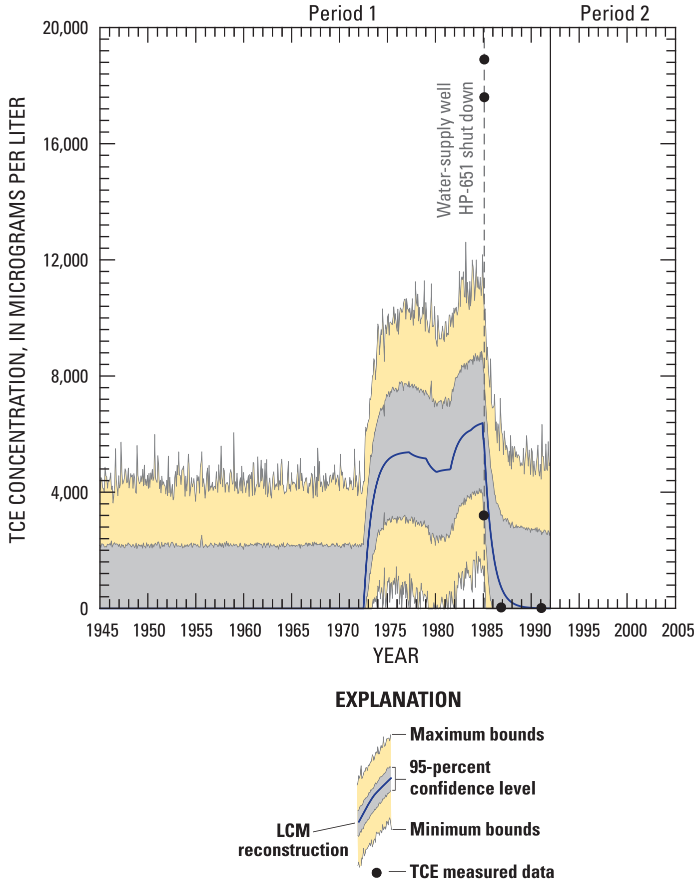


Figure S5.29. Linear control model results for reconstruction of trichloroethylene (TCE) concentration over time *(A)* at four selected locations, *(B)* at HP-651, with eight internal data points used in the analysis, and *(C)* at HP-651 with measured TCE data, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well locations]

Figure S5.30. Monte Carlo simulation results for maximum and minimum bounds and 95-percent confidence interval (2.5–97.5 percentile range) for trichloroethylene (TCE) concentration reconstructed at water-supply well HP-651, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well location]



LCM Results for *trans*-1,2-Dichloroethylene (1,2-tDCE) and Vinyl Chloride (VC)

The interim, step-wise determinations developed during the LCM process for 1,2-tDCE and VC are similar to those described for PCE and TCE. For brevity, only the final deterministic and stochastic results are presented in Figures S5.31 and S5.32 for 1,2-tDCE and VC, respectively.

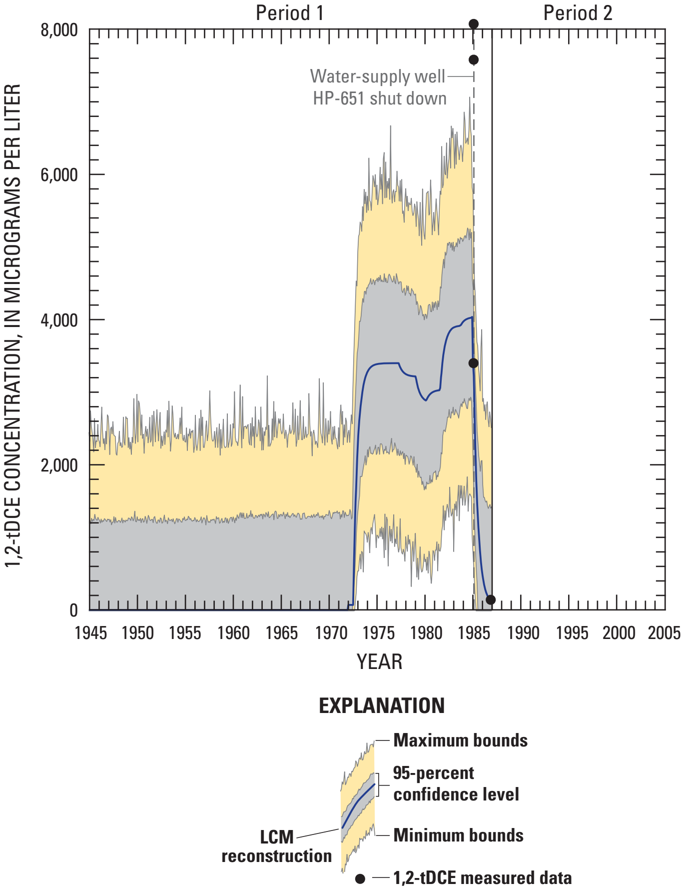


Figure S5.31. Monte Carlo simulation results for maximum and minimum bounds and 95-percent confidence interval (2.5–97.5 percentile range) for *trans*-1,2-dichloroethylene (1,2-tDCE) concentration reconstructed at water-supply well HP-651, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well location]

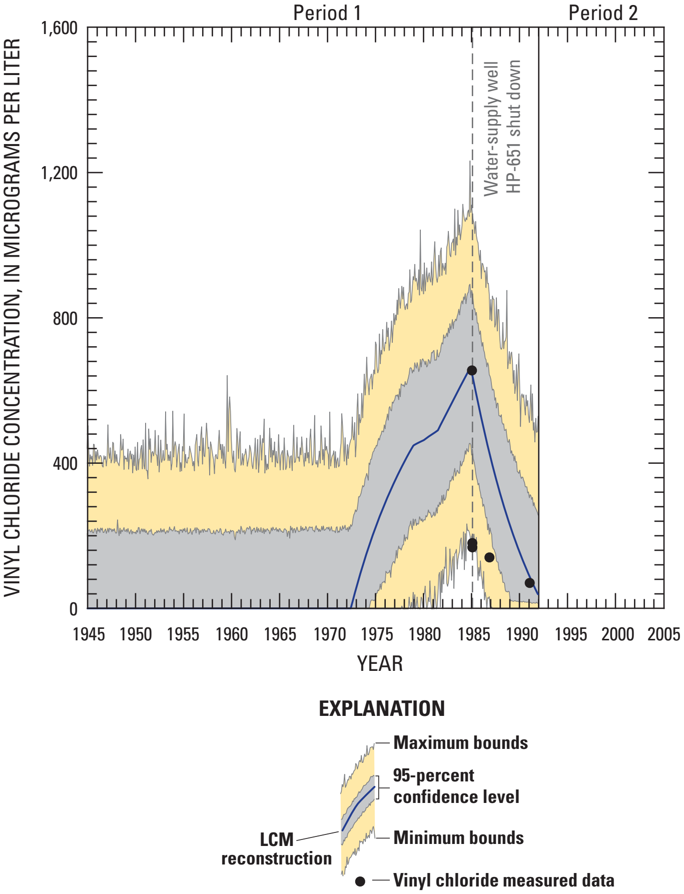


Figure S5.32. Monte Carlo simulation results for maximum and minimum bounds and 95-percent confidence interval (2.5–97.5 percentile range) for vinyl chloride concentration reconstructed at water-supply well HP-651, U.S. Marine Corps Base Camp Lejeune, North Carolina. [See Figure S5.23 for well location]

Discussion

For the LCM method verification at the Tarawa Terrace analysis area, both forward and backward time integration procedures as well as several different scenarios for available observation (measured) data are explored. An examination of the results indicates the following:

- The TCE history reconstructed using the LCM methodology for five selected observation locations within the Tarawa Terrace analysis area is consistent with the physical behavior of the groundwater flow system in this area. Additionally, the LCM results for TCE at each location are in good agreement with the results obtained using the previously developed numerical model for this analysis area.

- The contaminant history is reconstructed with greater accuracy at observation locations with relatively higher measured contaminant concentrations (i.e., observation locations 3, 4, and 5) than at observation locations with lower contaminant concentrations in groundwater (i.e., observation locations 1 and 2) (Figures S5.17–S5.19).

- The addition of internal data points (measured data available during Period 1 of the reconstruction) improves the accuracy of the historical reconstruction (Figures S5.17 and S5.18).

- The forward time integration procedure has a relatively large error for contaminant concentrations at the beginning of the historical reconstruction period (Period 1) due to the initial effect of the water-supply well pumping rates (Figures S5.17*B* and S5.17*C*). The backward time integration procedure may reduce this error (Figures S5.18*B* and S5.18*C*), but its overall accuracy is slightly lower than that of the forward procedure (Figure S5.19).

- The Kalman filter algorithm coupled with the Monte Carlo simulation incorporates modeling and measurement errors and provides information on the probability distributions of concentrations at the observation sites. For a given confidence level, it is possible to define confidence intervals, or corridors, for the historical reconstruction of contaminant concentration over time (Figures S5.20–S5.22).

At observation location 3, the minimum and maximum uncertainty bounds derived from 10,000 Monte Carlo realizations for the LCM results encompass the expected monthly contaminant concentration values (from the numerical model) 80% of the 408-month reconstruction period (January 1951–December 1994; Figure S5.20) At observation locations 4 and 5, the Monte Carlo maximum and minimum uncertainty bounds for the LCM results encompass the expected monthly contaminant concentration values during the entire reconstruction period (Figures S5.21 and S5.22).

Several observation locations are selected for application of the LCM method within the HPLF analysis area, but the primary focus is on reconstruction of contaminant history at water-supply well HP-651. The historical reconstruction at HP-651 is conducted for PCE, TCE, and their associated degradation products 1,2-tDCE and VC. Given the similarity in LCM results for the forward and backward time integration procedures at the Tarawa Terrace analysis, only the forward time integration procedure of the LCM method is used for the HPLF application. The LCM results indicate the following:

- The arrival time of all four contaminants at HP-651 is during July and August 1972. The arrival time for each contaminant is defined as when it exceeds its corresponding U.S. Environmental Protection Agency (USEPA) maximum contaminant level (MCL)[5]. The concentration of each of the contaminants increases rapidly during 1972–1975, remains more or less consistent during the late 1970s and early 1980s, and then decreases rapidly after HP-651 is shut down in February 1985. This profile corresponds to the operational period of water-supply well HP-651, which was put in service in July 1972 and taken out of service on February 4, 1985 (Figures S5.3 and S5.16). The contaminant concentrations in the vicinity of HP-651 are clearly controlled by the operation (pumping schedule) of HP-651. Site data indicate that (1) natural groundwater flow in this area is to the north/northwest, and (2) the contaminant source area is northwest of HP-651. Given these conditions, the contaminants would only reach HP-651 when it was actively pumping. When HP-651 is not pumping, groundwater flow and contaminant transport from the source area is naturally away from HP-651 and toward Wallace Creek (Figure S5.4).

---

[5] See Table A3 in Maslia et al. (2013) for a list of MCLs for the contaminants of interest in the Camp Lejeune study.

- All four contaminants reach their respective maximum concentrations at HP-651 in late 1984. A summary of the deterministic maximum concentration for each contaminant, as well as the 95% upper and lower confidence bounds (representing the 2.5–97.5 percentile range of Monte Carlo realizations) around the maximum, is included in Table S5.15.

- PCE, TCE, 1,2-tDCE, and VC are generally in good agreement with measured data available at HP-651 (Figure S5.24). Of note, two measured values of TCE (17,600 µg/L and 18,900 µg/L), collected on February 4, 1985, are significantly higher than the LCM results. However, a TCE measurement of 3,200 µg/L, recorded less than a month before on January 16, 1985, was an order of magnitude lower in concentration and within the uncertainty bounds associated with the LCM results. A physical explanation for the inordinately high TCE measured values on February 4, 1985, may be associated with the continuous operation of HP-651 for 14 days prior to the measurement date. As described in Faye et al. 2010 (pages C63–C64), the continuous operation of HP-651 during this time was atypical. In contrast, the January 16, 1985, TCE measurement occurred after HP-651 had been inactive for the previous 8 days. Given this physical scenario, all three TCE measurements collected on January 16 and February 4, 1985, may be valid and accurate. However, the January 16, 1985, measurement of 3,200 µg/L of TCE is likely more representative of typical operations.

- The maximum and minimum uncertainty bounds derived from 10,000 Monte Carlo realizations for the LCM results encompass most of the measured data values for each of the four contaminants (Figures S5.27, S5.30, S5.31, and S5.32). Of note, some of these measured data values were selected and used as internal data in the LCM solution, therefore close agreement with the model results is expected for those points.

- The uncertainty analyses for the LCM reconstruction of these contaminants yield (1) maximum and minimum uncertainty bounds based on 10,000 Monte Carlo realizations and (2) confidence bounds for a 95% confidence level representing the 2.5–97.5 percentile range of Monte Carlo realizations.

Overall, the reconstructed contaminant histories and the uncertainty bounds developed using the LCM approach may be useful in subsequent modeling, health risk assessment, and other health-related studies at the site.

As is true with modeling in general, the LCM method and associated results are an approximate representation of reality that should be considered carefully and within the context of the assumptions used when constructing and applying it. The primary limitations of the LCM application at the HPLF analysis area are the quality, scarcity, and temporal clustering of field data (measured data) for contaminants during the reconstruction period. The quality and general availability of measured data for the contaminants are the defining factors for the successful application and ultimate accuracy of the LCM application. A critical number of measured data points may allow application of the LCM method, but a shortage of internal data points during Period 1 of the reconstruction period can limit the accuracy of the reconstruction. As the LCM verification in the Tarawa Terrace analysis area demonstrated, the accuracy of the reconstruction is greatly improved as more internal data are included (Figures S5.17 and S5.18). The few measured data points that are available for use as internal points in the HPLF reconstruction are temporally clustered around the shutdown of HP-651. If additional measured data were available further back in time, the accuracy of not only the LCM method, but also any modeling effort seeking to reconstruct historical contaminant behavior, would be improved. Because the contaminant reconstruction in the HPLF analysis area is controlled by the operational (pumping) schedule at water-supply well HP-651, it is worth noting that this operational schedule is itself a reconstruction based on available historical records [Chapter A–Supplement 1 (Sautner et al. 2013), Chapter A–Supplement 2 (Telci et al. 2013)].

Table S5.15. Maximum concentrations and confidence bounds for linear control model reconstruction at water-supply well HP-651,Hadnot Point landfill (HPLF) analysis area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[µg/L, micrograms per liter; %, percent]

Contaminant	Maximum concentration, in µg/L	95% lower confidence bound	95% upper confidence bound	Date
Tetrachloroethylene (PCE)	413	245	575	12/1984
Trichloroethylene (TCE)	6,382	3,979	8,615	12/1984
trans-1,2-dichloroethylene (1,2-tDCE)	4,037	2,886	5,201	12/1984
Vinyl chloride	660	455	892	11/1984

Conclusions

The proposed LCM approach is verified using a numerical model previously developed for the Tarawa Terrace analysis area of USMCB Camp Lejeune. The historical contaminant concentration distributions developed using the LCM approach are consistent with the physical behavior of the groundwater system and are in good agreement with the contaminant fate and transport results of the previously developed numerical model. Contaminant history is reconstructed with greater accuracy at observation locations with relatively higher contaminant concentrations than at observation locations with lower contaminant concentrations. For the three observation locations with relatively higher contaminant concentrations, the range of relative average error is 4–32%.

The LCM approach is successfully applied to reconstruct the contaminant history of PCE, TCE, 1,2-tDCE, and VC at water-supply well HP-651 in the HPLF analysis area. The results are reasonable and consistent with available site data. Some of the key conclusions are as follows:

- The arrival time of PCE, TCE, 1,2-tDCE, and VC at HP-651 is during July and August 1972, corresponding to when HP-651 was placed in service. The arrival time for each contaminant is defined as when it exceeds its USEPA MCL[6]. The concentration of each of the contaminants increases rapidly during 1972–1975, remains more or less consistent during the late 1970s and early 1980s, and then decreases rapidly after HP-651 is shut down in February 1985. Contaminant transport in the vicinity of HP-651 is clearly controlled by the operation (pumping schedule) of HP-651.
- All four contaminants reach their respective maximum concentrations at HP-651 in late 1984 or early 1985.
- Deterministic LCM results indicate that the highest contaminant concentrations at HP-651 are for trichloroethylene (TCE), with a maximum concentration of 6,382 micrograms per liter (µg/L) occurring in December 1984. The corresponding confidence interval for the 95% confidence level is 3,979–8,615 µg/L of TCE.
- PCE, TCE, 1,2-tDCE, and VC are generally in good agreement with measured data available at HP-651

Successful verification and application of the LCM approach at the Tarawa Terrace and HPLF analysis areas, respectively, suggest that it is an encouraging companion, or possible alternative, to traditional numerical groundwater modeling methods. Because the LCM approach requires minimal system information and development time, it can be used early in a complex project to provide estimates for historical contaminant concentrations at selected observation locations. Combined with uncertainty analyses using Monte Carlo methods, the LCM method also can provide reasonable maximum and minimum bounds for historical reconstruction. Early in a project, this information may be valuable in decision-making, such as whether to pursue more complex model development, and also as a point of comparison for results of other modeling methods.

References

Ahlfeld D and Heidari M. Applications of Optimal Hydraulic Control to Ground-Water Systems. Journal of Water Resources Planning and Management. 1994;120(3):350–365.

Aliev FA, and Larin VB. Optimization of Linear Control Systems: Analytical Methods and Computational Algorithms. New York: Gordon and Breach Science Publishers; 1998.

Aral MM, Guan J, and Maslia ML. Identification of Contaminant Source Location and Release History in Aquifers. Journal of Hydrologic Engineering. 2001;6(3):225–234.

Atwood DF and Gorelick SM. Hydraulic Gradient Control for Groundwater Contaminant Removal. Journal of Hydrology. 1985;76(1–2):85–106.

Baker Environmental, Inc. Final Remedial Investigation Report for Operable Unit No. 2 (Sites 6, 9, and 82), Marine Corps Base Camp Lejeune, North Carolina; 1993. Contract Task Order 0133, Contract No.: N62470-89-D-4814 (CERCLA Administrative Record File #1272).

Björck, À. Numerical methods for least squares problems. Philadelphia: Society for Industrial and Applied Mathematics; 1996.

CH2M HILL, Inc. and Baker Environmental, Inc. Annual Monitoring Report, Operable Unit 2—Sites 6 & 82, Marine Corps Base Camp Lejeune, North Carolina, Reporting Period October 2001–December 2002; 2002. Contract Task Order 0120, Contract No.: N62470-95-D-6007 (CERCLA Administrative Record File #3278).

Culver TB and Shoemaker CA. Dynamic Optimal Control for Groundwater Remediation with Flexible Management Periods. Water Resources Research. 1992;28(3):629–641.

Engineering and Environment, Inc. and Michael Baker Jr., Inc. Annual Monitoring Report, Operable Unit 2—Sites 6 & 82, Marine Corps Base Camp Lejeune, North Carolina, Reporting Period January 2004–December 2004; 2005. Contract Task Order 0004, Contract No.: N62470-03-D-4000 (CERCLA Administrative Record File #3267).

---

[6] See Table A3 in Maslia et al. (2013) for a list of MCLs for the contaminants of interest in the Camp Lejeune study.

Environmental Science and Engineering, Inc. Characterization Step Report for Hadnot Point Industrial Area, Confirmation Study to Determine Existence and Possible Migration of Specific Chemicals In Situ, Marine Corps Base Camp Lejeune, North Carolina; 1988. Contract No.: N62470-83-C-6106 (CERCLA Administrative Record File #258).

Faye RE. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter B: Geohydrologic Framework of the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarawa Terrace Aquifer. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2012.

Faye RE, Anderson BA, Suárez-Soto RJ, and Sautner JB. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter C: Occurrence of Selected Contaminants in Groundwater at Installation Restoration Program Sites. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2010.

Faye RE, and Green JW Jr. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter E: Occurrence of Contaminants in Groundwater. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Faye RE, Jones LE, and Suárez-Soto RJ. Descriptions and Characterizations of Water-Level Data and Groundwater Flow for the Brewster Boulevard and Castle Hayne Aquifer Systems and the Tarawa Terrace Aquifer—Supplement 3. In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

Faye RE, and Valenzuela C. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter C: Simulation of Groundwater Flow. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Guan J, and Aral MM. Optimal Remediation with Well Locations and Pumping Rates Selected as Continuous Decision Variables. Journal of Hydrology. 1999;221(1):20–42.

Guan J, Kentel E, and Aral MM. Genetic Algorithm for Constrained Optimization Models and Its Application in Groundwater Resources Management. Journal of Water Resources Planning and Management. 2007;134(1):64–72.

Holland JH. Adaptation in Natural and Artificial Systems. Ann Arbor: University of Michigan Press; 1975.

Jang W and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter G: Simulation of Three-Dimensional Multispecies, Multiphase Mass Transport of Tetrachloroethylene (PCE) and Associated Degradation By-Products. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Jones L, Willis R, and Yeh WWG. Optimal Control of Nonlinear Groundwater Hydraulics Using Differential Dynamic Programming. Water Resources Research. 1987;23(11):2097–2106.

Maslia ML, editor. Expert Panel Assessing Methods and Analyses for Historical Reconstruction of Groundwater Resources and Distribution of Drinking Water at Hadnot Point, Holcomb Boulevard, and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina, April 29–30, 2009; *Prepared by* Eastern Research Group, Inc., Atlanta, GA: *Prepared for* Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.

Maslia ML, Sautner JB, Faye RE, Suárez-Soto RJ, Aral MM, Grayman WM, Jang W, Wang J, Bove FJ, Ruckart PZ, Valenzuela C, Green JW Jr, and Krueger AL. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter A: Summary of Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2007.

Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

National Research Council. Contaminated Water Supplies at Camp Lejeune—Assessing Potential Health Effects. Washington, DC: The National Academies Press; 2009.

Neupauer RM, Borchers B, and Wilson JL. Comparison of Inverse Methods for Reconstructing the Release History of a Groundwater Contamination Source. Water Resources Research. 2000;36(9):2469–2476.

Pardalos PM and Yatsenko VA. Optimization and Control of Bilinear Systems: Theory, Algorithms, and Applications. Springer Science + Business Media, LLC; 2008.

Sautner JB, Anderson BA, Suárez-Soto RJ, and Maslia ML. Descriptions and Characterizations of Data Pertinent to Water-Supply Well Capacities, Histories, and Operations—Supplement 1. In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

Skaggs TH and Kabala ZJ. Recovering the release history of a groundwater contaminant. Water Resources Research. 1994; 30(1):71–79.

Telci IT, Sautner JB, Suárez-Soto RJ, Anderson BA, Maslia ML, and Aral MM. Development and Application of a Methodology to Characterize Present-Day and Historical Water-Supply Well Operations—Supplement 2. In: Maslia ML, Suárez-Soto RJ, Sautner JB, Anderson BA, Jones LE, Faye RE, Aral MM, Guan J, Jang W, Telci IT, Grayman WM, Bove FJ, Ruckart PZ, and Moore SM. Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina—Chapter A: Summary and Findings. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2013.

Walpole RE, Myers RH, Myers SL, and Ye KE. Probability & Statistics for Engineers and Scientists. Pearson Prentice Hall; 2007.

Wang J, and Aral MM. Analyses of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water at Tarawa Terrace and Vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina: Historical Reconstruction and Present-Day Conditions—Chapter H: Effect of Groundwater Pumping Schedule Variation on Arrival of Tetrachloroethylene (PCE) at Water-Supply Wells and the Water Treatment Plant. Atlanta, GA: Agency for Toxic Substances and Disease Registry; 2008.

Zhou Y and van Geeralmod FC. KALMOD, a Stochastic-Deterministic Model for Simulating Groundwater Flow with Kalman Filtering. Hydrological Sciences Journal. 1992;37(4).

Table S5.3

Table S5.3. Selected wells in the vicinity of water-supply well HP-651 with reported analyses of tetrachloroethylene (PCE), trichloroethylene (TCE), 1,1-dichloroethylene (1,1-DCE), *trans*-1,2-dichloroethylene (1,2-tDCE), *cis*-1,2-dichloroethylene (1,2-cDCE), total 1,2-dichloroethylene (1,2-DCE), or vinyl chloride (VC), Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.

[SW, supply well; MW, monitor well; RW, remediation well; <, constituent is less than the detection limit. Number following the "<" is the detection limit; NA, constituent concentration not determined in laboratory analysis; D, sample diluted for analysis; ND, constituent not detected; J, estimated concentration; B, constituent detected in associated analytical method blank; E, value exceeds calibration range of the analytical equipment; R, analytical results rejected]

Well name	Well type	Sample date	Concentration, in micrograms per liter						
			PCE	TCE	1,1-DCE	1,2-tDCE	1,2-cDCE	Total 1,2-DCE	VC
HP-651	SW	1/16/85	386	3,200	187	3,400	NA	NA	655
	SW	2/4/85	400	18,900	<200	7,580	NA	NA	168
	SW	2/4/85	307	17,600	<200	8,070	NA	NA	179
	SW	11/12/86	45	32	7.0	140	NA	NA	140
	SW	1/22/91	53	13	2.0D	NA	NA	75	70
06-GW01D	MW	11/4/92	630	58,000J	ND	NA	NA	5,600J	ND
	MW	3/23/93	920	50,000	51	NA	NA	26,000	800J
	MW	10/27/97	1,600	140,000D	<1,000	NA	NA	36,000D	520J
	MW	1/15/98	2,000J	170,000	<5,000	NA	NA	36,000	<10,000
	MW	4/16/98	1,300J	110,000	<2,500	NA	NA	30,000	<5,000
	MW	7/23/98	1,200JD	110,000BD	47	NA	NA	24,000D	320E
	MW	1/16/99	390	180,000	72	7,600	18,000	NA	520
	MW	7/29/99	980JD	59,000D	35	3,800D	10,000D	14,000D	330E
	MW	1/18/00	990EJ	49,000D	32	3,300D	8,800D	12,000D	310E
	MW	7/30/00	880D	43,000	<5.0	6,200	16,000D	23,000D	360D
	MW	1/15/01	790D	49,000D	20	4,300D	11,000D	16,000D	91
	MW	7/18/01	6,500	48,000	21	3,200	8,000	11,000	110
	MW	1/15/02	210J	8,200	7.0	450	1,400	1,800	36
	MW	7/31/02	R	R	4.0J	R	R	R	14
	MW	1/24/03	<280	6,400	4.0J	230J	630	870	13
	MW	1/20/04	370JD	12,000D	5.0J	210JD	520D	730JD	10J
	MW	7/26/04	610JD	20,000D	9.0	560JD	1,700JD	NA	31
06-GW01DA	MW	5/3/93	2.9	160	<1.0	NA	NA	100	<1.0
	MW	10/24/97	<10	2.1J	<10	NA	NA	<10	<10
	MW	1/15/98	<5.0	0.93J	<5.0	NA	NA	<5.0	<10
	MW	4/16/98	<5.0	13	<5.0	NA	NA	2.3J	<10
	MW	1/15/99	<5.0	13	<5.0	<5.0	<5.0	NA	<5.0
	MW	1/13/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/15/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/15/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/31/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/24/03	<5.0	2.0J	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/20/04	<5.0	0.6J	<5.0	<5.0	<5.0	<10	<2.0
06-GW01DB	MW	10/24/97	<10	<10	<10	NA	NA	<10	<10
	MW	1/15/98	1.0J	<5.0	<5.0	NA	NA	<5.0	<10
	MW	4/16/98	<5.0	7.5	<5.0	NA	NA	<5.0	<10
	MW	1/15/99	<5.0	7.0	<5.0	<5.0	<5.0	NA	<5.0
	MW	1/19/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0

Table S5.3. Selected wells in the vicinity of water-supply well HP-651 with reported analyses of tetrachloroethylene (PCE), trichloroethylene (TCE), 1,1-dichloroethylene (1,1-DCE), *trans*-1,2-dichloroethylene (1,2-tDCE), *cis*-1,2-dichloroethylene (1,2-cDCE), total 1,2-dichloroethylene (1,2-DCE), or vinyl chloride (VC), Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[SW, supply well; MW, monitor well; RW, remediation well; <, constituent is less than the detection limit. Number following the "<" is the detection limit; NA, constituent concentration not determined in laboratory analysis; D, sample diluted for analysis; ND, constituent not detected; J, estimated concentration; B, constituent detected in associated analytical method blank; E, value exceeds calibration range of the analytical equipment; R, analytical results rejected]

Well name	Well type	Sample date	Concentration, in micrograms per liter						
			PCE	TCE	1,1-DCE	1,2-tDCE	1,2-cDCE	Total 1,2-DCE	VC
06-GW01DB	MW	1/10/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
Continued	MW	1/14/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/31/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/24/03	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/20/04	<5.0	<5.0	<5.0	<5.0	<5.0	<10	<2.0
06-GW01S	MW	11/19/86	<3.0	<3.0	<2.8	<1.6	NA	NA	<1.0
	MW	1/21/87	<3.0	<3.0	<2.8	<1.6	NA	NA	<1.0
	MW	6/27/91	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
	MW	10/24/92	2.9	1.0	ND	NA	NA	ND	ND
	MW	3/23/93	<1.0	<1.0	<1.0	NA	NA	<1.0	<1.0
	MW	10/24/97	12	<10	<10	NA	NA	<10	<10
	MW	1/15/98	2.8J	<5.0	<5.0	NA	NA	<5.0	<10
	MW	4/16/98	<5.0	1.4J	<5.0	NA	NA	<5.0	<10
	MW	7/24/98	9.3	<5.0	<5.0	NA	NA	<5.0	<10
	MW	1/15/99	6.0	<5.0	<5.0	<5.0	<5.0	NA	<5.0
	MW	7/28/99	2.0J	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/13/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/11/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/10/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/10/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/21/03	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/20/04	<5.0	<5.0	<5.0	<5.0	<5.0	<10	<2.0
	MW	7/26/04	<5.0	<5.0	<5.0	<5.0	<5.0	NA	<2.0
06-GW02DW	MW	6/27/91	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
	MW	11/3/92	1.4	ND	ND	NA	NA	ND	ND
	MW	3/21/93	<1.0	<4.0	<1.0	NA	NA	<1.0	<1.0
	MW	10/27/97	<10	<10	<10	NA	NA	<10	<10
	MW	1/17/98	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
	MW	4/18/98	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
06-GW02S	MW	11/20/86	<3.0	<3.0	<2.8	<1.6	NA	NA	<1.0
	MW	1/21/87	<3.0	<3.0	<2.8	<1.6	NA	NA	<1.0
	MW	1/19/91	<5.0	<5.0	<5.0	NA	NA	NA	<10
	MW	6/27/91	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
	MW	3/21/93	<1.0	<1.0	<1.0	NA	NA	<1.0	<1.0
06-GW15D	MW	5/3/93	1.0	34	<1.0	NA	NA	9.1	<1.0
	MW	7/26/97	<10	<10	<10	NA	NA	<10	<10
	MW	10/29/97	<10	<10	<10	NA	NA	<10	<10
	MW	1/19/98	<5.0	<5.0	<5.0	NA	NA	<5.0	<10

Table S5.3. Selected wells in the vicinity of water-supply well HP-651 with reported analyses of tetrachloroethylene (PCE), trichloroethylene (TCE), 1,1-dichloroethylene (1,1-DCE), *trans*-1,2-dichloroethylene (1,2-tDCE), *cis*-1,2-dichloroethylene (1,2-cDCE), total 1,2-dichloroethylene (1,2-DCE), or vinyl chloride (VC), Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[SW, supply well; MW, monitor well; RW, remediation well; <, constituent is less than the detection limit. Number following the "<" is the detection limit; NA, constituent concentration not determined in laboratory analysis; D, sample diluted for analysis; ND, constituent not detected; J, estimated concentration; B, constituent detected in associated analytical method blank; E, value exceeds calibration range of the analytical equipment; R, analytical results rejected]

Well name	Well type	Sample date	Concentration, in micrograms per liter						
			PCE	TCE	1,1-DCE	1,2-tDCE	1,2-cDCE	Total 1,2-DCE	VC
06-GW15D	MW	4/18/98	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
Continued	MW	1/17/99	<5.0	6.0	<5.0	<5.0	<5.0	NA	<5.0
	MW	1/18/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/11/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/15/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	8/1/02	<5.0	0.8J	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/24/03	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/20/04	<5.0	<5.0	<5.0	<5.0	<5.0	<10	<2.0
06-GW15S	MW	10/23/92	ND	1.9	ND	NA	NA	6.4	ND
	MW	3/21/93	<1.0	8.0	<1.0	NA	NA	6.4	<1.0
06-GW33	MW	3/18/93	<1.0	<1.0	<1.0	NA	NA	<1.0	<1.0
	MW	7/27/97	<10	<10	<10	NA	NA	<10	<10
	MW	10/24/97	5.0J	<10	<10	NA	NA	<10	<10
	MW	1/16/98	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
	MW	4/15/98	<5.0	0.96J	<5.0	NA	NA	<5.0	<10
	MW	7/25/98	13	<5.0	<5.0	NA	NA	<5.0	<10
	MW	1/15/99	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0
	MW	7/28/99	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/13/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/11/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/10/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/11/01	<5.0	120	<5.0	23	94	120	<2.0
	MW	1/14/02	6.0	180	<5.0	32	150	180	<2.0
	MW	7/29/02	<5.0	94	<5.0	11	54	66	<2.0
	MW	1/21/03	0.5J	88	<5.0	5.0J	30	35	<2.0
	MW	1/22/04	<5.0	6.0	<5.0	<5.0	0.4J	0.4J	<2.0
	MW	7/28/04	<5.0	5.0	<5.0	<5.0	0.5J	NA	<2.0
06-GW34	MW	3/18/93	1,200	610	1.3	NA	NA	410	<1.0
	MW	7/24/97	170J	310	<250	NA	NA	<250	<250
	MW	10/24/97	120	400	<100	NA	NA	170	<100
	MW	1/16/98	120	510	<25	NA	NA	200	<50
	MW	4/16/98	170D	250D	<5.0	NA	NA	130	<10
	MW	7/23/98	88JD	170D	<12	NA	NA	<64JD	<25
	MW	1/15/99	350	440	<5.0	56	110	NA	<5.0
	MW	7/28/99	4,100	470J	<500	<500	<500	<500	<200
	MW	1/12/00	560D	250D	<5.0	30	66	96	<2.0
	MW	7/11/00	6,000D	160	<5.0	19	140	160	<2.0
	MW	1/10/01	850D	200	<5.0	19	44	62	<2.0
	MW	7/11/01	380J	96	<5.0	21	36	57	<2.0

Table S5.3. Selected wells in the vicinity of water-supply well HP-651 with reported analyses of tetrachloroethylene (PCE), trichloroethylene (TCE), 1,1-dichloroethylene (1,1-DCE), *trans*-1,2-dichloroethylene (1,2-tDCE), *cis*-1,2-dichloroethylene (1,2-cDCE), total 1,2-dichloroethylene (1,2-DCE), or vinyl chloride (VC), Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[SW, supply well; MW, monitor well; RW, remediation well; <, constituent is less than the detection limit. Number following the "<" is the detection limit; NA, constituent concentration not determined in laboratory analysis; D, sample diluted for analysis; ND, constituent not detected; J, estimated concentration; B, constituent detected in associated analytical method blank; E, value exceeds calibration range of the analytical equipment; R, analytical results rejected]

Well name	Well type	Sample date	Concentration, in micrograms per liter						
			PCE	TCE	1,1-DCE	1,2-tDCE	1,2-cDCE	Total 1,2-DCE	VC
06-GW34	MW	1/14/02	1,800	100	<5.0	18	250	270	<2.0
Continued	MW	7/29/02	2,400	240	<5.0	33	200	280	<2.0
	MW	1/21/03	6,300	150	<5.0	13	160	180	<2.0
	MW	1/22/04	1,000D	33	<5.0	3.0J	41	44	<2.0
	MW	7/26/04	1,200D	34	<5.0	3.0J	30	NA	<2.0
06-GW40DA	MW	10/28/97	<10	<10	<10	NA	NA	<10	<10
	MW	1/18/98	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
	MW	4/17/98	<5.0	4.4J	<5.0	NA	NA	<5.0	<10
06-GW40DW	MW	7/24/97	<10	<10	<10	NA	NA	<10	<10
	MW	10/28/97	<10	<10	<10	NA	NA	<10	<10
	MW	1/18/98	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
	MW	4/17/98	<5.0	<5.0	<5.0	NA	NA	<5.0	<10
	MW	1/18/99	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0
	MW	1/19/00	<5.0	14	<5.0	<5.0	4.0J	4.0J	<2.0
	MW	1/15/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/15/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	8/1/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/24/03	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/22/04	<5.0	0.6J	<5.0	<5.0	<5.0	<10	<2.0
06-GW41	MW	1/15/99	<5.0	9.0	<5.0	<5.0	<5.0	<5.0	<5.0
	MW	7/29/99	<5.0	3.0J	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/12/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/11/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/10/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/11/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/14/02	<5.0	<5.0	<5.0	<5.0	3.0J	3.0J	<2.0
	MW	7/29/02	6.0	17	<5.0	11	24J	35	<2.0
	MW	1/21/03	<5.0	2.0J	<5.0	<5.0	3.0J	3.0J	<2.0
	MW	1/23/04	<5.0	<5.0	<5.0	<5.0	<5.0	<10	<2.0
	MW	7/26/04	<5.0	0.7J	<5.0	<5.0	0.6J	NA	<2.0
06-GW42	MW	1/15/99	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0
	MW	1/12/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/11/00	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/10/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/11/01	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/14/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	7/29/02	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/21/03	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	MW	1/22/04	<5.0	<5.0	<5.0	<5.0	0.6J	0.6J	<2.0
	MW	7/26/04	<5.0	0.3J	<5.0	<5.0	0.4J	NA	<2.0

Table S5.3. Selected wells in the vicinity of water-supply well HP-651 with reported analyses of tetrachloroethylene (PCE), trichloroethylene (TCE), 1,1-dichloroethylene (1,1-DCE), *trans*-1,2-dichloroethylene (1,2-tDCE), *cis*-1,2-dichloroethylene (1,2-cDCE), total 1,2-dichloroethylene (1,2-DCE), or vinyl chloride (VC), Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[SW, supply well; MW, monitor well; RW, remediation well; <, constituent is less than the detection limit. Number following the "<" is the detection limit; NA, constituent concentration not determined in laboratory analysis; D, sample diluted for analysis; ND, constituent not detected; J, estimated concentration; B, constituent detected in associated analytical method blank; E, value exceeds calibration range of the analytical equipment; R, analytical results rejected]

Well name	Well type	Sample date	Concentration, in micrograms per liter						
			PCE	TCE	1,1-DCE	1,2-tDCE	1,2-cDCE	Total 1,2-DCE	VC
82-MW30	MW	3/22/93	<1.0	1.5J	<1.0	NA	NA	<1.0	<1.0
82-DRW01	EW	4/17/98	1,300	35,000D	<500	NA	NA	9,300	<500
	EW	7/28/98	1,400	36,000	<1,000	NA	NA	10,000	<2,000
	EW	10/19/98	<2,000	24,000	<2,000	NA	NA	4,900	<2,000
	EW	1/15/99	790J	21,000	29	990J	2,900	NA	120
	EW	4/17/99	1,200D	27,000D	19	2,000D	5,400D	NA	95
	EW	7/28/99	1,700	31,000	<1,000	2,300	5,700	8,000	<400
	EW	10/23/99	2,500D	71,000D	19	3,400	9,000D	7,300	64
	EW	1/17/00	2,400D	35,000D	20	3,000D	7,400D	10,000D	87
	EW	7/13/00	1,600D	25,000D	19	2,700D	5,700D	7,700D	77
	EW	1/10/01	3,800D	36,000D	15	3,400D	9,300D	13,000D	54
	EW	7/10/01	4,600J	34,000	18	4,000	11,000	15,000	69
	EW	1/15/02	1,400	15,000	12	1,100	3,100	4,200	60
	EW	1/27/03	1,200	14,000	10	1,200	2,800	4,000	41
	EW	1/22/04	740D	9,600D	8.0	960D	2,200D	NA	27
	EW	7/26/04	860D	11,000D	6.0J	790D	2,000D	NA	20J
82-DRW04	EW	4/16/98	<620	20,000	<620	NA	NA	7,600	<620
	EW	7/28/98	150J	21,000	<1,000	NA	NA	7,700	<2,000
	EW	10/19/98	<1,000	21,000	<1,000	NA	NA	6,300	<1,000
	EW	1/15/99	1,100	15,000	34	1,100	2,800	NA	240
	EW	4/17/99	56	17,000D	17J	1,600	4,400D	NA	130
	EW	7/29/99	79	22,000D	16	1,800D	5,000D	6,100D	110
	EW	10/23/99	99	24,000D	18	3,000D	7,700D	6,600	110
	EW	1/17/00	110	33,000D	19	3,300D	7,600D	11,000D	140
	EW	7/13/00	130	17,000D	18	1,700D	4,700D	6,400D	130
	EW	1/10/01	140	9,000D	18	3,300D	8,400D	12,000D	100
	EW	7/11/01	490J	22,000	82	2,700	7,600	10,000	120
	EW	1/15/02	200	9,300	15	1,000	2,600	3,600	98
	EW	7/31/02	190	R	14	R	R	R	60
	EW	1/27/03	1,900	8,400	18	950	2,300	3,200	79
	EW	1/22/04	180	6,700D	13	920D	2,100D	NA	68
	EW	7/26/04	190	6,000D	16	570D	1,500D	NA	40
82-SRW01	EW	4/22/98	560	1,600	<50	NA	NA	620	<100
	EW	7/23/98	680D	2,300BD	<120	NA	NA	1,100D	<120
	EW	10/19/98	360	850D	<50	NA	NA	230	<50
	EW	1/15/99	680	770	<5.0	89	170	NA	<5.0
	EW	4/17/99	1,100	530	<50	61	150	NA	<50
	EW	1/17/00	2,400D	1,600D	2.0J	180	550D	790D	<2.0

Table S5.3. Selected wells in the vicinity of water-supply well HP-651 with reported analyses of tetrachloroethylene (PCE), trichloroethylene (TCE), 1,1-dichloroethylene (1,1-DCE), *trans*-1,2-dichloroethylene (1,2-tDCE), *cis*-1,2-dichloroethylene (1,2-cDCE), total 1,2-dichloroethylene (1,2-DCE), or vinyl chloride (VC), Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[SW, supply well; MW, monitor well; RW, remediation well; <, constituent is less than the detection limit. Number following the "<" is the detection limit; NA, constituent concentration not determined in laboratory analysis; D, sample diluted for analysis; ND, constituent not detected; J, estimated concentration; B, constituent detected in associated analytical method blank; E, value exceeds calibration range of the analytical equipment; R, analytical results rejected]

Well name	Well type	Sample date	Concentration, in micrograms per liter						
			PCE	TCE	1,1-DCE	1,2-tDCE	1,2-cDCE	Total 1,2-DCE	VC
82-SRW01	EW	7/13/00	2,100JD	3,600D	3.0J	570E	2,500JD	2,500JD	<2.0
Continued	EW	1/10/01	2,900D	1,200D	<5.0	62	150	210	<2.0
	EW	7/10/01	1,600	920J	<5.0	82	200	280	<2.0
	EW	1/15/02	300J	5,500	11	1,700	4,300	6,000	3.0
	EW	7/31/02	2,100	1,800	<250	400	1,100J	1,500J	<100
	EW	1/27/03	1,900	1,200	3.0J	380J	870	1,200	0.5J
	EW	1/22/04	1,900D	190D	0.6J	32	100	140	<2.0
	EW	7/26/04	3,900D	320D	<5.0	55	160	NA	<2.0
82-SRW02	EW	4/22/98	28	230	<10	NA	NA	190	<20
	EW	7/28/98	28	280	<12	NA	NA	410	<25
	EW	1/15/99	8.0	30	<5.0	6.0	25	NA	<5.0
	EW	4/17/99	6.0	90	<5.0	33	100	NA	2.0J
	EW	10/25/99	1,100D	24,000D	25	3,300D	8,700D	7,500	160
	EW	1/17/00	18	74	<5.0	20	71	91	<2.0
	EW	7/13/00	75	840JD	<5.0	200E	920JD	920JD	15
	EW	1/10/01	3.0J	<5.0	<5.0	<5.0	<5.0	<5.0	<2.0
	EW	7/18/01	14	140	<5.0	54	150	200	4.0
	EW	1/15/02	18	140	<5.0	60	160	220	8.0
	EW	1/27/03	26	250	0.6J	120	260	340	25
	EW	1/22/04	150	310D	1.0J	170	340D	490D	13
	EW	7/26/04	43	90	<5.0	28	75	NA	1.0J
82-SRW03	EW	4/22/98	130	1,600	<100	NA	NA	1,500	<100
	EW	7/28/98	100	1,200	<50	NA	NA	1,500	<100
	EW	10/19/98	350	2,100	<100	NA	NA	1,500	<100
	EW	1/15/99	180	520	<5.0	270	860	NA	22
	EW	4/17/99	220D	1,300D	2.0J	430D	1,100D	NA	10
	EW	7/28/99	370	2,900	<100	940	2,900	3,800	50
	EW	10/23/99	21	110	<5.0	27	99	120	<2.0
	EW	1/17/00	210	1,400	<50	460	1,200	1,700	25
	EW	7/13/00	72	2,200D	<5.0	660D	2,700D	3,300D	NA
	EW	1/15/01	66	1,500D	<5.0	640D	1,400D	1,700D	18
	EW	7/10/01	62	400	<5.0	160	2,000	2,500	11
	EW	1/15/02	53	520	<5.0	160	780	850	16
	EW	7/31/02	18	R	1.0J	86	R	R	8.0
	EW	1/27/03	50	350	2.0J	120	540	670	23
	EW	1/22/04	42	510D	2.0J	230D	790D	1,000D	21
	EW	7/26/04	58	530D	2.0J	190	700D	NA	22

Table S5.3. Selected wells in the vicinity of water-supply well HP-651 with reported analyses of tetrachloroethylene (PCE), trichloroethylene (TCE), 1,1-dichloroethylene (1,1-DCE), *trans*-1,2-dichloroethylene (1,2-tDCE), *cis*-1,2-dichloroethylene (1,2-cDCE), total 1,2-dichloroethylene (1,2-DCE), or vinyl chloride (VC), Hadnot Point landfill analysis area, Hadnot Point–Holcomb Boulevard study area, U.S. Marine Corps Base Camp Lejeune, North Carolina.—Continued

[SW, supply well; MW, monitor well; RW, remediation well; <, constituent is less than the detection limit. Number following the "<" is the detection limit; NA, constituent concentration not determined in laboratory analysis; D, sample diluted for analysis; ND, constituent not detected; J, estimated concentration; B, constituent detected in associated analytical method blank; E, value exceeds calibration range of the analytical equipment; R, analytical results rejected]

Well name	Well type	Sample date	Concentration, in micrograms per liter						
			PCE	TCE	1,1-DCE	1,2-tDCE	1,2-cDCE	Total 1,2-DCE	VC
82-SRW04	EW	4/23/98	360	2,800	<170	NA	NA	2,100	<330
	EW	7/28/98	190	1,400	<100	NA	NA	1,100	<200
	EW	10/19/98	87	650	<50	NA	NA	720	<50
	EW	1/15/99	86	960	<5.0	280	1,500	NA	79
	EW	4/17/99	80	450D	<10	90	350	NA	7.0J
	EW	7/29/99	560	1,100D	<50	410	1,300	1,700	25
	EW	10/23/99	82	6,500D	7.0	990D	6,100D	3,200	74
	EW	1/17/00	130	570D	<5.0	97	340D	430D	12
	EW	7/13/00	87	550D	<5.0	91	310D	390D	16
	EW	1/10/01	57	550D	<5.0	94	320D	390D	12
	EW	7/10/01	56	1,100	<5.0	60	720	880	9.0
	EW	1/15/02	49	180	<5.0	55	180	210	11
	EW	7/31/02	29	R	0.4J	29	180	210	5.0
	EW	1/27/03	43	260	1.0J	50	210	310	9.0
	EW	1/22/04	36	320D	1.0J	72	290D	410D	15
	EW	7/26/04	14	310D	0.9J	44	240D	NA	9.0

ATSDR
AGENCY FOR TOXIC SUBSTANCES
AND DISEASE REGISTRY

Analyses and Historical Reconstruction of Groundwater Flow, Contaminant Fate and Transport, and Distribution of Drinking Water Within the Service Areas of the Hadnot Point and Holcomb Boulevard Water Treatment Plants and Vicinities, U.S. Marine Corps Base Camp Lejeune, North Carolina— Chapter A–Supplement 5: Theory, Development, and Application of Linear Control Model Methodology to Reconstruct Historical Contaminant Concentrations at Selected Water-Supply Wells