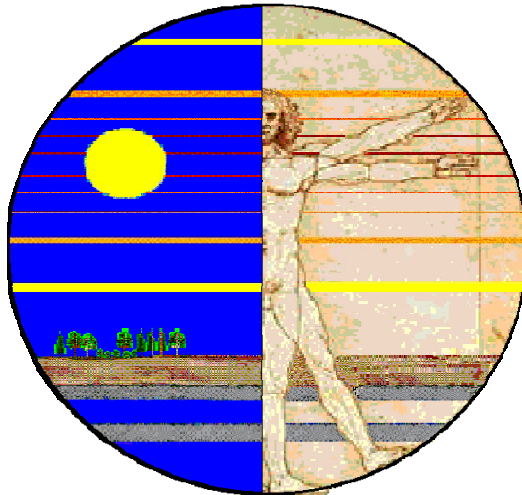


**EFFECT OF GROUNDWATER PUMPING SCHEDULE
VARIATION ON ARRIVAL OF
TETRACHLOROETHYLENE (PCE) AT WATER-SUPPLY
WELLS AND THE WATER TREATMENT PLANT**

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Jinjun Wang and Mustafa M. Aral

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Research report No.: MESL-01-07; January 2007, 91p.**

Keywords – Groundwater, Exposure-dose reconstruction, hydrogeology, coupled simulation-optimization model.

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Glossary of Acronyms and Abbreviations

ATSDR:	Agency for Toxic Substances and Disease Registry
CEE:	School of Civil and Environmental Engineering
DIS:	Discretization file for MODFLOW
FTL:	Flow-transport link
GA:	Genetic algorithm
GT:	Georgia Institute of Technology
KTC:	Kuhn-Tucker condition
Max. Sche.:	Pumping schedule yielding the early arrival time
Min. Sche. I:	Pumping schedule yielding the late arrival time with no conditions on the well TT-26 schedules
Min. Sche. II:	Pumping schedule yielding the late arrival time with conditions on the well TT-26 schedules
MCL:	Maximum contaminant level
MESL:	Multimedia Environmental Simulations Laboratory
OBS:	Concentration observation file for MT3DMS
Org. Sche.	Original pumping schedule used by ATSDR
PCE	Tetrachloroethylene
PSOpS:	Pumping Schedule Optimization System
S/O:	Simulation optimization
USGS:	U.S. Geological Survey
WEL:	Well package for MODFLOW
WTP:	Water treatment plant

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Abstract

The Agency for Toxic Substances and Disease Registry (ATSDR) is conducting an epidemiological study to evaluate whether exposures (in-utero and during infancy – up to 1 year of age) to volatile organic compounds that contaminated the drinking water at the U.S. Marine Corps Base Camp Lejeune, North Carolina, were associated with specific birth defects and childhood cancers that are observed at the site. The study includes the births that occurred to women who were pregnant while they resided in the family housing at the base during the period 1968 – 1985. There is no exposure data and very limited site-specific contamination data are available to support the epidemiological study. As a result, ATSDR is using modeling techniques to estimate the historical and present-day contamination conditions in the groundwater and the water treatment plant at Camp Lejeune, North Carolina. Owing to the complexity of the historical reconstruction process, a number of reports are being prepared to provide a comprehensive description of information and data used in historical reconstruction and present-day analyses at Tarawa Terrace and vicinity. To complement these studies, this report describes the effect of groundwater pumping schedule variations on the arrival times of Tetrachloroethylene (PCE) at water-supply wells and the water treatment plant (WTP).

During the historical reconstruction study, as described in various ATSDR reports accompanying this report, the groundwater flow and fate-and-transport of contaminants in the Tarawa Terrace area of the Camp Lejeune base and its vicinity have been simulated to evaluate the contaminant concentration in the WTP. Due to the uncertainty residing in the reconstructed input data used in these simulations, uncertainty may be present in the simulated contaminant concentrations in the water-supply wells and the WTP, hence the times for contaminant concentrations to reach the maximum contaminant level (MCL) at these locations. A major cause and contributor to this uncertainty is the pumping schedules used in the ATSDR model, therefore, in this study the focus is on the uncertainty associated with the pumping schedules. The study included the development of a simulation and optimization (S/O) procedure identified as PSOpS (Pumping Schedule Optimization System), which combines simulation models and optimization

techniques to optimize the pumping schedules for maximum or minimum contaminant concentrations in the WTP. Based on the optimized pumping schedules, variations of PCE concentration and the maximum contaminant level (MCL, 5 ppb for PCE) arrival time at water-supply wells and the WTP are evaluated. The results of this study indicate that the variation of pumping schedules may cause significant changes in the contaminant concentration levels and MCL arrival time at the WTP.

1 Introduction

The Agency for Toxic Substances and Disease Registry (ATSDR) is conducting an epidemiological study to evaluate whether exposures (in-utero and during infancy up to 1 year of age) to volatile organic compounds (VOC) that contaminated drinking water at the U.S. Marine Corps Base Camp Lejeune, North Carolina, were associated with specific birth defects and childhood cancers. To provide the epidemiological study with quantitative estimates of exposure, characterization of environmental contamination and the frequency and duration of exposure to contaminated drinking water is being conducted using the historical reconstruction process [Maslia et al., 2001].

The site investigation at the base concluded that groundwater was the sole source of water to the WTP. The contaminant source was the ABC One-Hour Cleaners located in the Tarawa Terrace area, and the major contaminants at the site included Tetrachloroethylene (PCE) and its degradation by-products. Contaminants released from the ABC One-Hour Cleaners migrated into the groundwater system and eventually into the WTP through several water-supply wells in the Tarawa Terrace area of the base.

Based on the study of the hydrogeologic and the historical data from the Tarawa Terrace area and its vicinity, the ATSDR modeling team has reconstructed and simulated the multilayer groundwater flow at the site using MODFLOW, a groundwater flow simulation model [McDonald and Harbaugh, 1988]. The simulation model MT3DMS [Zheng and Wang, 1999] was then used to evaluate the fate-and-transport of contaminants in the subsurface. Based on this analysis, the concentration distribution and the arrival time of contaminants in the WTP were determined historically.

Due to its nature, the historical reconstruction modeling process conducted by ATSDR has uncertainties associated with it. These uncertainties could have a significant effect on the epidemiological study. One uncertainty is associated with the pumping schedules used in groundwater flow simulations because there are limited historical records of the pumping rates at the water-supply wells. In this study, the focus is on the evaluation of the uncertainty caused by the pumping schedules and its effect on the simulation results. For this purpose, a methodology was developed to yield the earliest/latest contaminant arrival times at the water-supply wells and the Tarawa Terrace WTP associated with the allowable variations in groundwater pumping schedules throughout the historical operation of the site. As it was developed in this study, this methodology uses a combination of simulations and optimization methods to adjust the pumping schedules while maintaining the historical total pumping demands at the Tarawa Terrace WTP that were identified by the ATSDR modeling team. The study presented here includes the following assumptions:

- i. Tetrachloroethylene (PCE) is the only contaminant of concern at the site, although other contaminants such as degradation by-products of PCE existed in the groundwater and at the WTP. In this study, the use of the term “contaminant”

- implies PCE, unless otherwise specified;
- ii. Pumping schedule is the only variable considered to be uncertain in this analysis. Some other factors, such as hydrogeologic variables, may also cause variations in contaminant transport process and may affect the contaminant concentration and arrival time at the water-supply wells and the WTP. The uncertainties associated with these variables are treated in other parallel studies conducted by ATSDR, and, therefore, are not considered in this study.

This study used two simulation models:

- i. **MODFLOW**: MODFLOW is a three-dimensional groundwater simulation model, which can be used in the solution of governing equations of multilayer groundwater flow systems. The model uses the finite-difference method in this process [McDonald and Harbaugh, 1984]. The model is developed by U. S. Geological Survey and is an open source code. MODFLOW-2000 (also identified as MF2K), a fourth generation of MODFLOW, is employed in this study. In this report, all MODFLOW related information was adopted from the report authored by Harbaugh et al. [2000] unless otherwise identified. The executable file and the source codes of MODFLOW were downloaded from:
<http://water.usgs.gov/nrp/gwsoftware/modflow2000/modflow2000.html>;
- ii. **MT3DMS**: MT3DMS is a modular three-dimensional multispecies contaminant transport model. It can be used in the simulation of advective, diffusive, and reactive transport of contaminants in multilayer groundwater systems [Zheng and Wang, 1999]. All the MT3DMS related information in this report was obtained from the reports authored by Zheng and Wang [1999] and Zheng [2005] unless otherwise identified. The version of MT3DMS model employed in this study is version 5.1. The executable file and the source codes of MT3DMS were downloaded from the website at: <http://hydro.geo.ua.edu/mt3d/>.

In this study, all information regarding the Camp Lejeune Marine Corps Base and the input data used for the models previously described above were obtained from ATSDR. Details of the framework and the basis of the data can be found in other ATSDR reports, and will not be discussed in detail here.

The organization of this report is as follows. In Chapter 2, a review of the study conducted by the ATSDR modeling team is provided, including a review of the background and the simulation models used in the historical reconstruction study. A groundwater simulation and optimization procedure, identified as PSOpS (Pumping Schedule Optimization System), developed by the researchers at Multimedia Environmental Simulations Laboratory (MESL), Georgia Tech (GT), is introduced in Chapter 3. The simulation results and a discussion of these results are presented in Chapter 4, which is followed by a summary section in Chapter 5.

2 A Review of ATSDR Camp Lejeune Study

2.1 Background

The Agency for Toxic Substances and Disease Registry (ATSDR), U. S. Department of Health and Human Services, is currently (2007) conducting a historical reconstruction of contaminant occurrences in water-distribution networks at Marine Corps Base Camp Lejeune, North Carolina. Camp Lejeune is located in the Coastal Plain of North Carolina, in Onslow County, southeast of the City of Jacksonville and about 70 miles northwest of the city of Wilmington, North Carolina. The purpose of this study is to determine if there is an association between the exposure to contaminated drinking water and the birth defects and the childhood cancers in children born to women who lived at the base while they were pregnant during the period 1968 to 1985.

Due to limited exposure data available for the period of interest (1968 – 1985), ATSDR has undertaken a reconstruction of the historical data. ATSDR's investigation focuses on the Tarawa Terrace area and its vicinity (Figure 2.1). The Tarawa Terrace area is bounded on the east by Northeast Creek, and to the south by New River and Northeast Creek. On the west and north, it is bounded by the drainage boundaries of these streams. The historical reconstruction includes the groundwater system reconstruction, contaminant source characterization, and contaminant fate-and-transport simulation in the groundwater system and the water distribution system serving the Tarawa Terrace area.

The ATSDR study concluded that groundwater was the sole source of water to the WTP and water distribution system serving the Tarawa Terrace area. The source of contaminants in the groundwater was the ABC One-Hour Cleaners located to the north of several water-supply wells at Tarawa Terrace (Figure 2.1). According to the ATSDR study, Tetrachloroethylene (PCE) was continuously released to the subsurface system at a rate of 1,200 gram/day during the period January 1953 to December 1984. PCE released from ABC One-Hour Cleaners migrated into the groundwater system and was then pumped into the WTP by the water-supply wells shown in Figure 2.1.

Using the reconstructed hydrogeologic data and the contaminant source characterization, the ATSDR modeling team was able to simulate the groundwater flow and contaminant fate-and-transport in the subsurface system of the Tarawa Terrace area to obtain the historical exposure data. Due to the nature of historical reconstruction, uncertainties are associated with the reconstructed data, which will in turn cause uncertainties in the resulting exposure data. The uncertainties in the exposure outcome may have a significant effect on the epidemiological study. In particular, the uncertainty caused by the groundwater pumping schedule used in the simulations has been pointed out to be important. Therefore, in this study, there is an evaluation of the variation in PCE concentrations and the arrival time of maximum contaminant level (MCL, 5 ppb for PCE) at the water-supply wells and the WTP that could be caused by the variation of groundwater pumping rates at the water-supply wells.

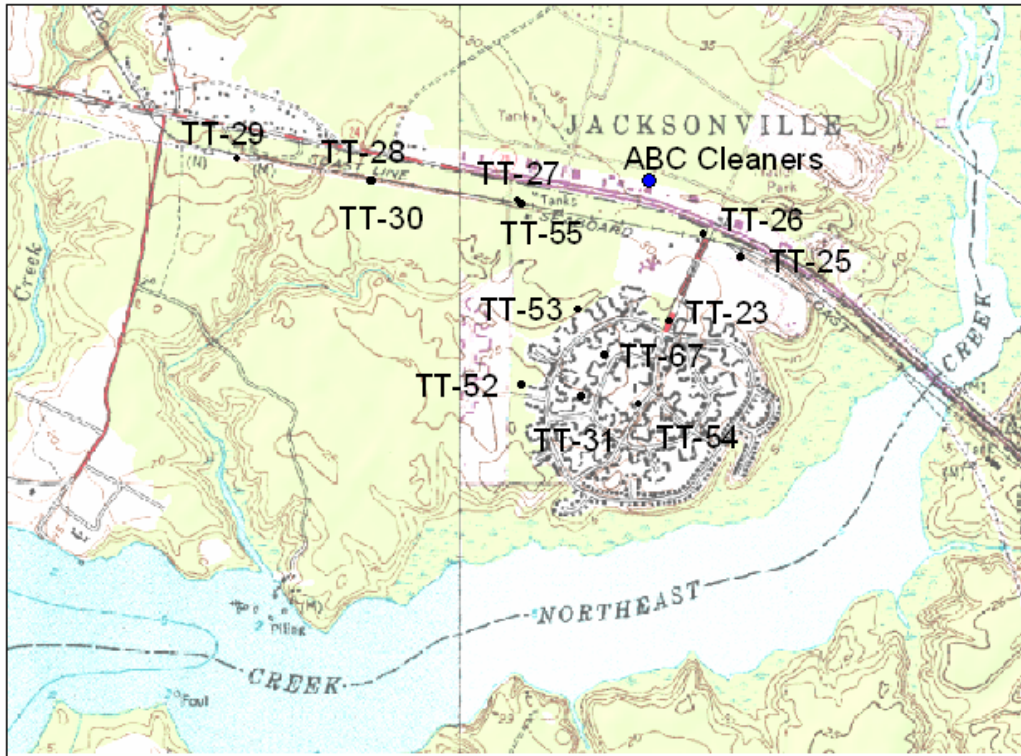


Figure 2.1. Water-supply well locations at Tarawa Terrace and vicinity, U.S. Marine Corps Base Camp Lejeune, North Carolina.

2.2 Introduction to simulation tools and input data

In the ATSDR study, the contaminant concentration in the WTP was evaluated by employing the following steps:

- i. MODFLOW model was used to simulate the groundwater flow in the Tarawa Terrace area and its vicinity. The MODFLOW simulation also generated the flow-transport link (FTL) file to be used in the MT3DMS simulation;
- ii. Using the FTL file, along with other input files, MT3DMS simulation was conducted to obtain the contaminant concentrations in the water-supply wells; and,
- iii. The contaminant concentration distribution obtained from MT3DMS simulation was used to calculate the PCE concentration in the WTP through a volumetric mixing model.

In the following sections, MODFLOW and MT3DMS models and their input files are briefly described, as they are used in the ATSDR study and this study.

2.2.1 MODFLOW model and input data

MODFLOW is a computer program that was designed to solve the three-dimensional equation, Equation (2.1), governing groundwater flow by using the finite-difference

method [McDonald and Harbaugh, 1988] for both steady state and transient flow applications:

$$\frac{\partial}{\partial x}(K_{xx} \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y}(K_{yy} \frac{\partial h}{\partial y}) + \frac{\partial}{\partial z}(K_{zz} \frac{\partial h}{\partial z}) + W = S_s \frac{\partial h}{\partial t} \quad (2.1)$$

in which K_{xx} , K_{yy} , and K_{zz} are hydraulic conductivity values along the x -, y -, and z -coordinate axis directions (L/T); h is the piezometric head (L); W is a volumetric flux per unit volume that represents sources and/or sinks at the site (T^{-1}); S_s is the specific storage of the porous medium (L^{-1}); t is time (T); and x , y , z are the Cartesian coordinate directions (L).

MODFLOW was originally developed by McDonald and Harbaugh [1984]. Since then it has been modified numerous times, and several versions exist in the literature. The second version is identified as MODFLOW-88 [McDonald and Harbaugh, 1988], the third version is identified as MODFLOW-96 [Harbaugh and McDonald, 1996a and 1996b]. The latest version, which is used in this study, is identified as MODFLOW-2000 [Harbaugh et al., 2000]. Also since its inception, the following authors – Prudic [1989], Hill [1990], Leake and Prudic [1991], Goode and Appel [1992], Harbaugh [1992], McDonald et al. [1992], Hsieh and Freckleton [1993], Leake et al. [1994], Fenske et al. [1996], Leake and Lilly [1997], and Hill et al. [2000] – have made several improvements to MODFLOW.

In the ATSDR study, as well as this study, MODFLOW model was applied to generate the flow-transport link (FTL) file for the MT3DMS simulation. In addition, MODFLOW is also a component of the newly developed PSOpS model.

In MODFLOW simulations, a fundamental component of the time discretization data is the “time step.” A group of time steps are identified as a “stress period” [Harbaugh et al., 2000]. In this study, from the first month of year 1951 through the last month of year 1994, each month is identified as a stress period, and there are a total of 528 stress periods in the overall simulation period. January of 1951 is “stress period 1,” February is “stress period 2,” and so forth. Within a stress period, the time dependent variables, such as the groundwater pumping rates of pumping wells, are constant, therefore, the update of the pumping schedule, as reconstructed in this study, occurs monthly.

In MODFLOW the basic spatial simulation unit used in the finite-difference calculations is called a “finite-difference cell” or “cell.” In the ATSDR study, the groundwater system in the Tarawa Terrace area and its vicinity is modeled as a zone that contains 200 rows, 270 columns, and 7 layers of cells. In other words, a total of 378,000 cells are used to idealize the three-dimensional groundwater flow region at the site.

The input data for the MODFLOW simulation can be divided into two categories: (i) “global process input” data file and, (ii) “groundwater flow process input” data file. Global process input files contain basic information that is applied to the whole

simulation. As for the groundwater flow process input files, a group of related input data are put together into a file as the input for a specific “package.” For example, discretization (DIS) file is a global process input file. It contains data such as number of rows, columns and layers in the model, cell widths etc. In comparison to that, the well (WEL) file is a file that contains input data for the “Well Package,” including the locations and pumping rates of water-supply wells in each stress period. Based on these types of classifications, the MODFLOW input files, as used in the ATSDR study, are given below and are summarized in Table 2.1.

There are two global process files used in the study:

- i. **File type:** NAM
File contents: The name and Fortran unit of each file used in the simulation;
- ii. **File type:** DIS
File contents: Basic discretization information, including number of rows, columns, and layers of the model; number of stress periods; confining layers information; width of each cell along rows and columns; elevation of each cell; period length, number of time steps, and the state (steady or transient) of each stress period.

The following nine groundwater flow process files are also used in the study:

- i. **File type:** BAS6
Package: Basic Package
File contents: Boundary conditions; piezometric head value in inactive cells; initial head distribution;
- ii. **File type:** BCF6
Package: Block-Centered Flow Package
File contents: Wet-dry cell information; layer type information (whether the layer is confined or not, and how the interblock transmissivity will be calculated); transmissivities or hydraulic conductivities; horizontal anisotropy factors; primary and secondary storage coefficients; vertical hydraulic conductivities divided by thickness of cells;
- iii. **File type:** DRN
Package: Drain Package
File contents: Number of drain parameters; maximum number of drain cells used in any stress period; number of parameters used in each stress period; location and elevation of each drain cell, and factors used to calculate the drain conductance in that cell;
- iv. **File type:** GHB
Package: General-Head Boundary Package
File contents: Number of general-head boundary parameters; maximum number of general-head-boundary cells used in any stress period; number of parameters used in each stress period; location of each constant head cell, and the heads in

- the cell at the beginning and end of each stress period;
- v. **File type:** OC
Package: Output Control Option
File contents: Information on whether the computed head, drawdown and water budget will be saved for each stress period; where to save and in what format;
 - vi. **File type:** PCG
Package: Preconditioned Conjugate-Gradient Package
File contents: Maximum number of outer and inner iterations; matrix conditioning method; head change criterion and residual criterion for convergence; relaxation parameter; printout interval;
 - vii. **File type:** RCH
Package: Recharge Package
File contents: Recharge distribution type; recharge flux (if applicable);
 - viii. **File type:** LMT6
Package: Link-MT3DMS Package [Zheng et al., 2001]
File contents: The name, unit, header, and format of the flow-transport link (FTL) file for MT3DMS simulation;
 - ix. **File type:** WEL
Package: Well Package
File contents: Maximum number of operating wells in each stress period; number, location and pumping rate of each well in each stress period.

Table 2.1. Input files used for the MODFLOW simulation code

Process	File Type	Package
Global	NAM	N/A
	DIS	N/A
Groundwater Flow	BAS6	Basic
	BCF6	Block-Centered Flow
	DRN	Drain
	GHB	General-Head Boundary
	OC	Output Control Option
	PCG	Preconditioned Conjugate-Gradient
	RCH	Recharge
	LMT6	Link-MT3DMS
	WEL	Well

2.2.2 MT3DMS model and input data

MT3DMS is a modular three-dimensional multi-species transport model that can be used in the simulation of advective, dispersive, and reactive transport of contaminants in groundwater flow systems [Zheng et al., 2001]. In the MT3DMS model, three major classes of transport solution techniques are applied so that the best approach can be offered for various transport problems for efficiency and accuracy. These three techniques include: the standard finite-difference method, the particle-tracking-based

Eulerian-Lagrangian methods, and the higher-order finite-volume total-variation-diminishing method.

The governing equation used in the MT3DMS simulation model can be given as:

$$\frac{\partial(\theta C^k)}{\partial t} = \frac{\partial}{\partial x_i}(\theta D_{ij} \frac{\partial C^k}{\partial x_j}) - \frac{\partial}{\partial x_i}(\theta v_i C^k) + q_s C_s^k + \sum R_n \quad (2.2)$$

where θ is the porosity of subsurface system; C^k is the concentration of species k in aqueous phase (ML^{-3}); t is time (T); x_i and x_j are the distances along the three-dimensional Cartesian coordinate axis directions (L); D_{ij} is the dispersion coefficient (L^2T^{-1}); v is pore velocity (LT^{-1}); q_s is the flow rate per unit volume of aquifer representing sinks and sources (T^{-1}); C_s^k is the concentration of species k in sink or source flux (ML^{-3}); and $\sum R_n$ is the chemical reaction term ($\text{ML}^{-3}\text{T}^{-1}$).

In the ATSDR study, as well as this study, MT3DMS is used to simulate the fate-and-transport of PCE in the groundwater system of the Tarawa Terrace area and its vicinity. The output of MT3DMS simulation provides PCE concentration in the water-supply wells.

Similar to the input files of MODFLOW, the input files of MT3DMS include one name file and some other input files used for various packages. These input files are described below and in Table 2.2.

- i. **File type:** NAM
File contents: The name and Fortran unit of each file employed in the simulation;
- ii. **File type:** BTN
Package: Basic Transport Package
File contents: Basic model information (number of rows, columns, layers, and stress periods); number of chemical species; transport and solution options; confining layer properties; cell width along rows and columns of each cell; porosity in each cell; boundary condition information; starting concentrations of each chemical species (initial conditions); printing options; output frequency; number of observation points and their locations; mass balance output options; and stress period information;
- iii. **File type:** ADV
Package: Advection Package
File contents: Advection solution option; and other advective transport simulation variables, if applicable;
- iv. **File type:** DSP
Package: Dispersion Package
File contents: Longitudinal dispersivities; ratio of horizontal transverse dispersivity to longitudinal dispersivity; ratio of vertical transverse dispersivity to

- longitudinal dispersivity; effective molecular diffusion coefficients;
- v. **File type:** SSM
Package: Sink and Source Mixing Package
File contents: Sink and source term options; maximum number of sinks and sources; concentration read-in options; concentration of evapotranspiration flux (if applicable); concentration in specified cells;
- vi. **File type:** RCT
Package: Chemical Reaction Package
File contents: Type of reaction; type of kinetic reaction; bulk densities of the aquifer medium for each cell; porosities of immobile domain (if applicable); initial concentration of the sorbed phase (if applicable); sorption parameters; reaction rates;
- vii. **File type:** GCG
Package: Generalized Conjugate-Gradient Solver Package
File contents: Maximum numbers of inner and outer iterations; relaxation factor; convergence criterion;
- viii. **File type:** FTL
Package: Flow-Transport Link Package
File contents: The groundwater flow related information.

Table 2.2. Input files used for the MT3DMS simulation code

File Type	Package
NAM	N/A
BTN	Basic Transport
ADV	Advection
DSP	Dispersion
SSM	Sink and Source Mixing
RCT	Chemical Reaction
GCG	Generalized Conjugate-Gradient Solver
FTL	Flow-Transport Link

2.2.3 Water-supply well information

The purpose of this study is to examine the effect of the updated pumping schedules on the PCE concentration and 5 ppb arrival time at the water-supply wells and the WTP. In this study, among all the input data used in the ATSDR study, only the groundwater pumping rates of the water-supply wells are considered to be uncertain and are varied based on an optimization procedure developed in this study. Therefore, it is necessary to present more detailed information about the water-supply system in the Tarawa Terrace area.

In the ATSDR study, a total of 16 water-supply wells were used to supply groundwater to the Tarawa Terrace WTP. Thirteen of these wells are located in the Tarawa Terrace area and its vicinity (Figure 2.1). The other three wells, identified as well 6, well 7, and well

TT-45, are located outside of this area and, therefore, are not shown in Figure 2.1. In both the ATSDR study and this study, it is assumed that well 6, well 7, and well TT-45 had zero contaminant concentration, which implies that these wells contributed only water but no contaminant mass to the WTP.

In MODFLOW and MT3DMS simulations, the location of a pumping well is identified in terms of the coordinates of the cell in which the well lies (x , y , z). In the simulation codes the x , y , and z values correspond to the layer number, row number, and column number of the cells respectively. According to the well-construction logs, some wells penetrate more than one layer of aquifer, therefore in MODFLOW simulations some well discharges are split into two or more “virtual” wells which extract water from different layers. For example, in the MODFLOW input used by the ATSDR, well TT-52 is split into TT-52A and TT-52B, where the extension “A” refers to Layer-1 and “B” refers to Layer-3. Wells TT-31 and TT-54 also are split this way. In this study well TT-53 and TT-67 are split to satisfy their pumping capacities, with respect to dry- and wet-cell conditions observed at the cell. Locations and service periods of these water-supply wells are listed in Table 2.3.

Table 2.3. Locations and service periods of water-supply wells in the Tarawa Terrace area

Well	Layer	Row	Column	Start Date	End Date
TT-23	3	84	175	08/1984	04/1985
TT-25	3	67	194	01/1982	02/1987
TT-26	3	61	184	01/1952	01/1985
TT-27	3	52	135	01/1952	12/1961
TT-28	3	47	96	01/1952	12/1971
TT-29	3	41	61	01/1952	06/1958
TT-30	3	47	97	01/1972	01/1985
TT-31A	1	104	152	01/1973	02/1987
TT-31B	3	104	152	01/1973	02/1987
TT-52A	1	101	136	01/1962	02/1987
TT-52B	3	101	136	01/1962	02/1987
TT-53A	1	81	151	01/1962	01/1984
TT-53B	3	81	151	01/1962	01/1984
TT-54A	1	106	167	01/1962	02/1987
TT-54B	3	106	167	01/1962	02/1987
TT-55	1	53	136	01/1962	12/1971
TT-67A	1	93	158	01/1972	02/1987
TT-67B	3	93	158	01/1972	02/1987

During the simulation period (1951 – 1994), the pumping rates of the water-supply wells varied, and some wells were out of service for some stress periods. Using the historical records, the pumping rates and the pumping capacities of each water-supply well were

generated for all the stress periods.

2.3 Simulation results of ATSDR modeling study

Using input files listed in Table 2.1, a MODFLOW simulation was performed to generate the flow-transport link (FTL) file for the follow-up MT3DMS simulation. The PCE concentration distribution in the water-supply wells was then obtained from an output file of MT3DMS simulation, the concentration observation (OBS) file, and these results are shown in Figure 2.2.

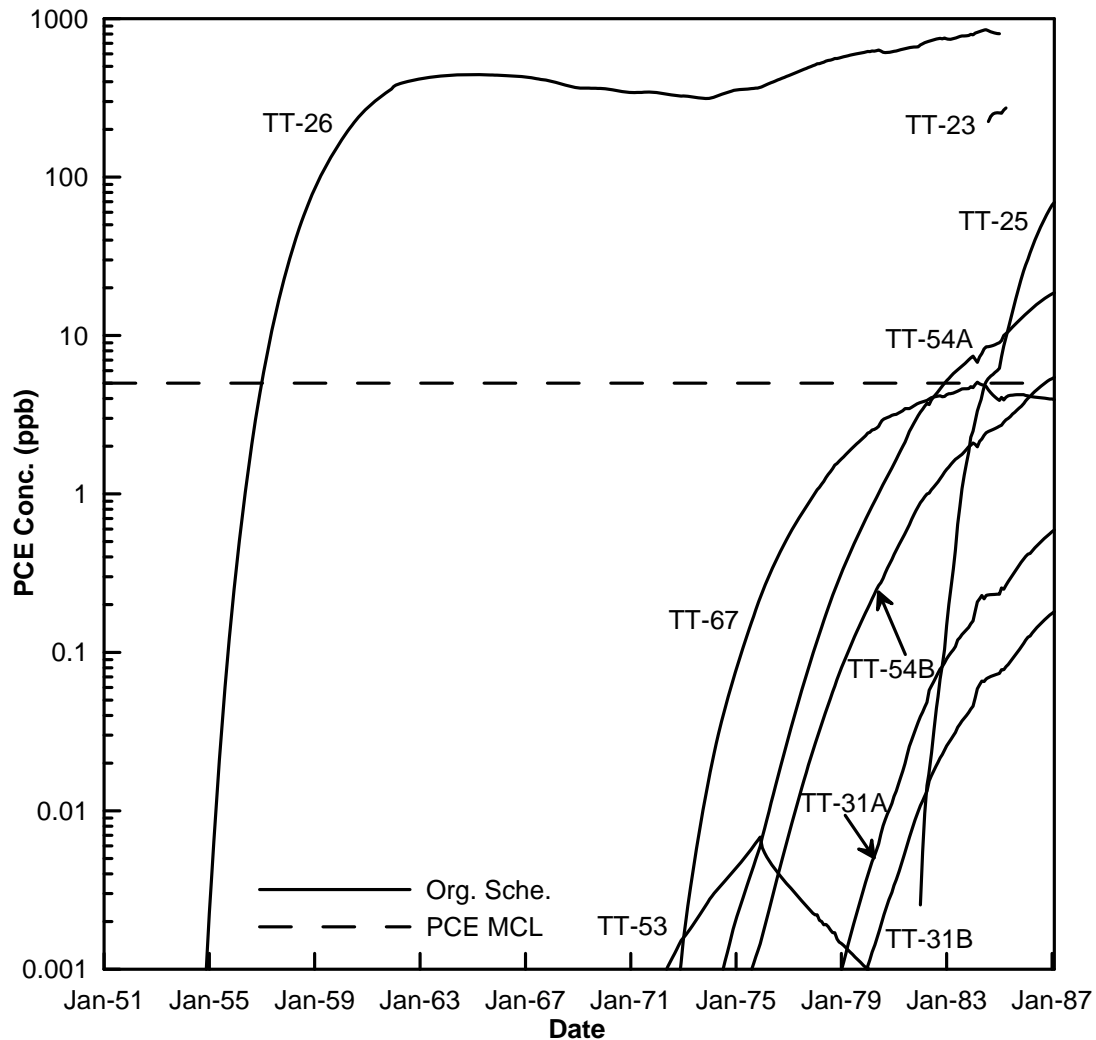


Figure 2.2. PCE concentrations in water-supply wells under the Original Schedule

In Figure 2.2 the PCE concentrations in the water-supply wells are shown during their service periods as listed in Table 2.3. Although 16 pumping wells were operating in the Tarawa Terrace area in ATSDR's simulation, only wells TT-26, TT-23, TT-25, TT-67, TT-54A and TT-54B had PCE concentrations higher than the MCL. Among them, well TT-26 had a much longer period of exposure to PCE concentrations over 5 ppb – the PCE MCL arrival time in well TT-26 is January 1957, while the second-earliest PCE

MCL arrival in a water-supply well occurred during January 1983 at well TT-54A. PCE concentration in well TT-26 is always much higher than in the other water-supply wells, indicating that TT-26 conveyed the majority of PCE mass introduced into the WTP. This is probably because of proximity of well TT-26 to the contaminant source and the well's long pumping history.

Employing the PCE concentration data in the water-supply wells, along with the pumping rates in these wells, the PCE concentration in the Tarawa Terrace WTP was calculated by using the following mixing model:

$$C_i = \frac{\sum_{j=1}^n q_{ij} c_{ij}}{Q_{Ti}} \quad (2.3)$$

in which C_i is the PCE concentration in the WTP at stress period i (ML^{-3}); n is the total number of active water-supply wells in stress period i ; q_{ij} is the pumping rate of well j at stress period i (L^3T^{-1}); c_{ij} is the PCE concentration in the water-supply well j at stress period i (ML^{-3}); and Q_{Ti} is the total water demand at stress period i (L^3T^{-1}).

The PCE concentration in the Tarawa Terrace WTP is shown in Figure 2.3. To distinguish it from other updated pumping schedules that were developed and are discussed in later chapters, the pumping schedule used in the ATSDR study is identified as the “Original Schedule” (Org. Sche.) in the figures as well as throughout the remainder of this report.

According to Figure 2.3, the PCE concentration in the Tarawa Terrace WTP first exceeded the MCL in November 1957. When this outcome is compared to the results presented in Figure 2.2, only well TT-26 had a PCE concentration over 0.001 ppb by November 1957. Therefore, well TT-26 is critical in assessing the PCE MCL arrival time in the WTP.

As shown in Figure 2.4, for the period of interest (January 1968 – December 1985), the maximum PCE concentration in the WTP is 183.04 ppb and the minimum PCE concentration is 0.72 ppb. During this period, however, there are only 15 months when the PCE concentration in the WTP is lower than 46.69 ppb. Therefore, for most of the period of interest (201 months out of 216 months), the PCE concentration in the Tarawa Terrace WTP ranges between 46.69 ppb and 183.04 ppb, and the average PCE concentration is about 86.39 ppb, which is much higher than the 5 ppb MCL for PCE.

The time periods in which the PCE concentration in the WTP is lower than 46.69 ppb are: July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985. These also are the time periods during which well TT-26 was out of service. As can be seen in Figure 2.2, during these time periods, the PCE concentrations in other water-supply wells were much lower than those in well TT-26. Stopping well TT-26 from supplying water to the WTP therefore caused the sudden PCE concentration drops as shown in Figure 2.3 and Figure 2.4.

For the PCE concentration drop at the end of 1961 in Figure 2.3, the reason is similar to the one described previously. At that time, the pumping rate of well TT-26 decreased from 28,715 ft³/day to 18,959 ft³/day, while the total water supplied to the WTP kept unchanged (116,199 ft³/day). Since the PCE concentrations in the other water-supply wells were negligible (less than 0.001 ppb) and the well TT-26 was the only source of PCE in the WTP at that time, a decrease of PCE concentration is expected in the WTP.

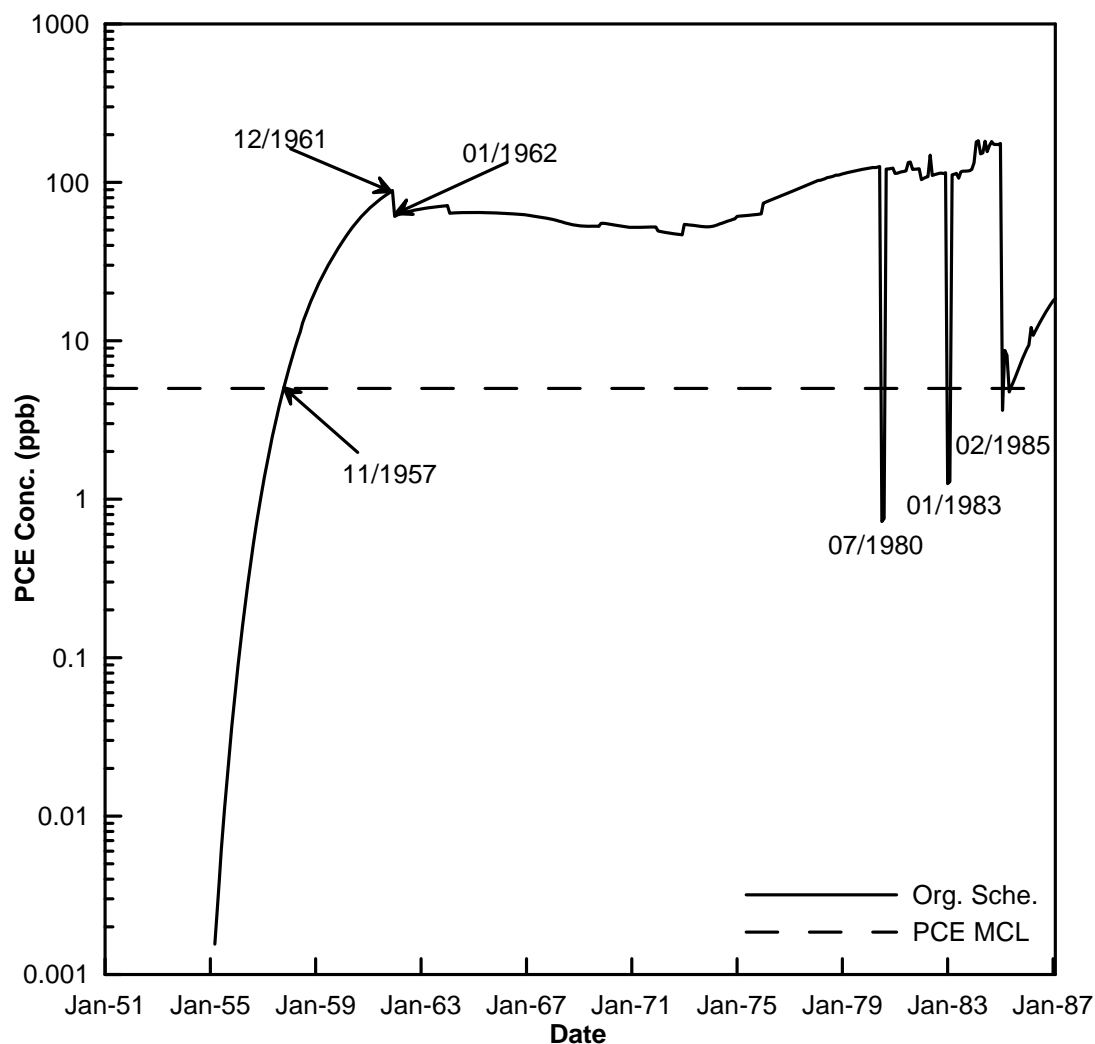


Figure 2.3. PCE concentrations in the WTP under the Original Schedule

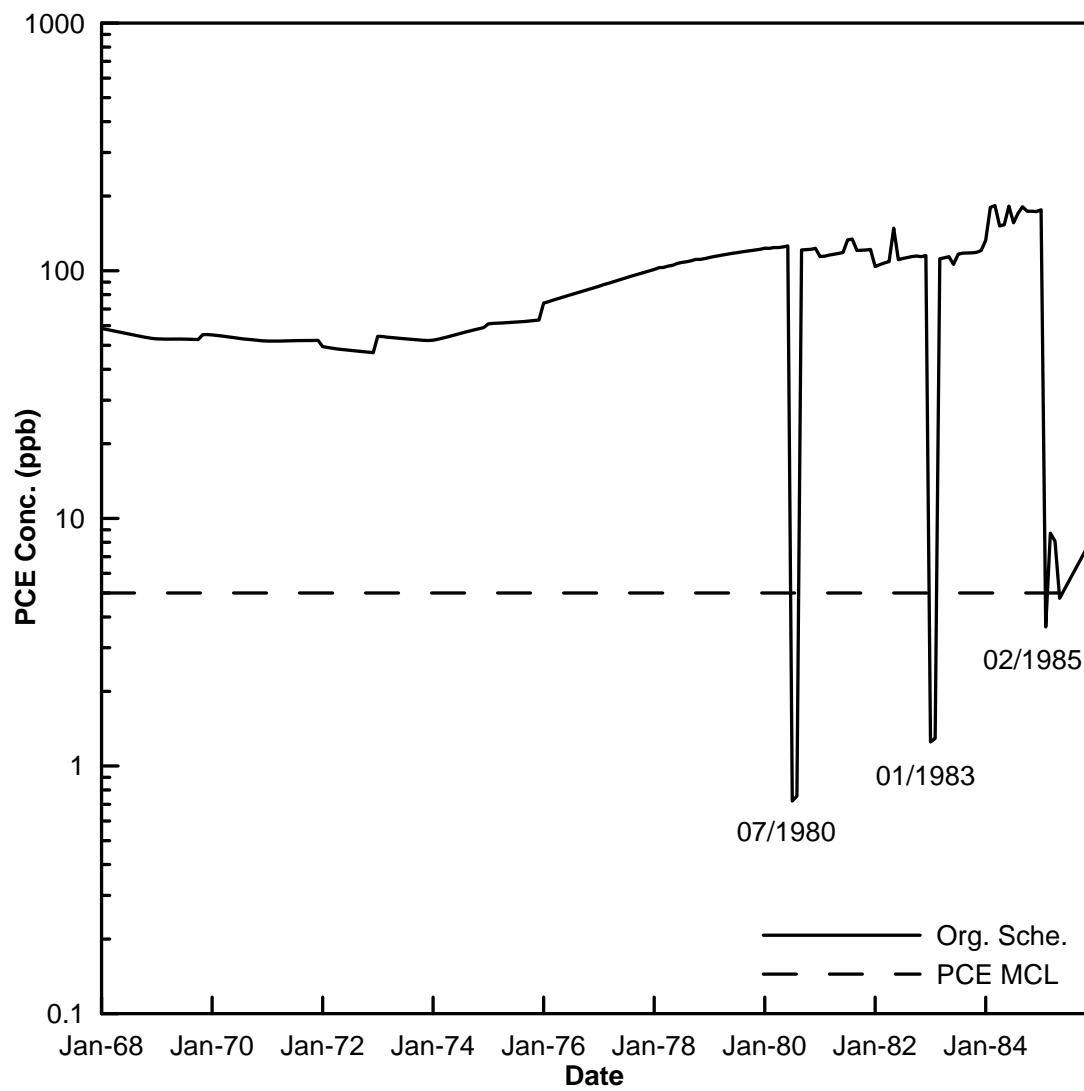


Figure 2.4. PCE concentrations in the WTP under the Original Schedule for the period of interest

3 Optimization of the Pumping Schedules

As introduced in Chapter 2, the PCE concentration in the Tarawa Terrace WTP was obtained through consecutive application of the following three steps:

- i. Simulation of groundwater flow using the MODFLOW model;
- ii. Simulation of PCE fate-and-transport using the MT3DMS model; and
- iii. Calculation of PCE concentration in the WTP using the MT3DMS output, the pumping schedules, and the WTP mixing model.

Throughout these steps, pumping schedules are used both in MODFLOW simulation and during the calculation of PCE concentration in the WTP when the mixing model is used. Moreover, as stated earlier, pumping schedules are the only uncertain variables in this study. Therefore, to evaluate the change in PCE arrival time at the water-supply wells and the WTP, pumping schedules that may cause that change must be obtained first according to certain criteria. In this study, a pumping schedule optimization procedure, identified as PSOpS (Pumping Schedule Optimization System), is developed using the simulation/optimization (S/O) approach. In PSOpS, the simulation models (MODFLOW and MT3DMS) are combined with optimization techniques to generate the optimal pumping schedules that would yield the “earliest” or the “latest” PCE MCL arrival times at the WTP.

3.1 Formulation of the optimization model

To evaluate the PCE arrival time at the WTP caused by a variation of pumping schedules, models must be identified to link the contaminant arrival time and the pumping schedules. Currently, several simulation models (or a combination of simulation models), which may be used in this analysis, are available in the literature.

Among the models, one straight forward choice is the combination of MODFLOW and MODPATH [Pollock, 1994]. MODPATH is a particle tracking model that computes the three-dimensional pathlines and the particle arrival times at the pumping wells based on the advective transport output of MODFLOW. A combination of MODFLOW and MODPATH can provide contaminant arrival time at the water-supply wells. However, several limitations in the MODPATH model restrict its use in this study. First, MODPATH only simulates the advective transport of contaminants in the groundwater system. In a MODPATH simulation, the advection of water is considered to be the only driving force of contaminant movement, while other factors which may also affect the movement of contaminants, such as diffusion and dispersion, are not considered. Second, in a MODPATH simulation, the contaminant is treated as a tracer, which implies no chemical reaction or degradation that maybe associated with the contaminant can be accounted for. Finally, although MODPATH simulation can provide contaminant arrival time at a pumping well, this time is only recorded for the first contaminant particle that arrives at the well. No concentration information is associated with this simulation output.

In this study, however, a more precise simulation of contaminant fate-and-transport is required, and the time for contaminant concentration that reaches a specific level is required for exposure evaluation purposes. Considering all these restrictions, the combination of MODFLOW and MT3DMS was selected for this study.

As introduced in the previous sections, MT3DMS is a subsurface contaminant fate-and-transport simulation model. Using the FTL file obtained from MODFLOW, the MT3DMS can be run on the same groundwater system. MT3DMS does not have the restrictions associated with the MODPATH model. The output file of MT3DMS provides contaminant concentrations at specified times and locations. Using this information, the arrival time at the water-supply wells of certain concentration levels can be evaluated. Other benefits of the coupled simulation of MODFLOW and MT3DMS include:

- i. By using the output of MT3DMS, the contaminant concentration in the WTP also can be calculated and evaluated; and,
- ii. By using the combination of MODFLOW and MT3DMS, all the original input files obtained from the ATSDR study can be applied directly and only a few complementary files need to be added within the PSOpS framework.

The following steps are used to evaluate the change of PCE arrival time caused by variations in pumping schedules:

- i. Optimize the pumping schedules for the “earliest” and the “latest” PCE arrival times using a combination of simulation models (MODFLOW and MT3DMS) and optimization techniques (S/O);
- ii. Simulate the groundwater flow and the contaminant fate-and-transport at the site using the optimal pumping schedules obtained from step (i);
- iii. Calculate PCE concentration at the WTP using Equation (2.3) and the optimal pumping schedules; and,
- iv. Evaluate the “earliest” and the “latest” PCE arrival times at the WTP.

In step (i), the optimization of pumping schedule for the “earliest” or the “latest” PCE arrival time is equivalent to optimizing the pumping schedule for the “maximum” or “minimum” PCE concentrations in the WTP because the observation of a higher concentration at the WTP implies an earlier contaminant arrival time, and vice versa. To optimize the pumping schedule for maximum or minimum PCE concentrations in the WTP, one approach is to optimize the pumping schedules for the maximum or minimum PCE concentrations for each stress period individually. After the maximum or minimum concentrations are obtained for each stress period, a relationship can be obtained between maximum or minimum concentration versus stress period (time). This approach, however, is associated with significant computational burden. The large scale of the simulation model – 200 rows, 270 columns, 7 layers, and 528 stress periods – clearly indicates that this approach will require a high end PC computer years of calculation time to complete the simulations and, therefore, is unacceptable.

Another possible approach is to combine the stress periods with same characteristics (pumping rates, pumping capacities, pumping demands, recharge, and so forth) together to reduce the size of the overall model. This approach, however, will lose some detail during optimization, which implies that it may not be as precise as the original model, and, thus, may affect the optimization results.

Considering the computation power and memory of the desktop workstations available for this study (64 bit dual processor PC boxes), along with the need to obtain an acceptable result in a timely manner without losing any detail and accuracy, the optimization problem needs to be formulated in a more computationally cost-efficient manner. To create such a model, the following observations were made about the site data used in these simulations:

- i. The contaminant was continuously released from the same source point;
- ii. Well TT-26 was the only major contaminant contributor to the Tarawa Terrace WTP; and,
- iii. Well TT-26 was in operation during most of the period of interest.

With these observations in mind, the optimization problem is reformulated as follows. Optimize each successive stress period i for a “maximum” or “minimum” PCE concentration in the WTP in stress period i while keeping all of the previously optimized pumping rates constant. In other words, in the reformulation, the pumping schedule of stress period 1 is first optimized for optimal (maximum or minimum) PCE concentration in the WTP in stress period 1. Then the pumping schedule of stress period 2 is optimized for optimal PCE concentration in stress period 2 keeping the optimization results from stress period 1 constant, and so on. In this manner, at the end of the simulation/optimization process an optimal pumping schedule, under which the PCE concentration in the WTP can be maximized or minimized, is obtained for all the stress periods.

The reformulated optimization problem for maximum PCE concentration in the WTP can be expressed mathematically as:

$$\begin{aligned}
 & \underset{q_i \in R^n}{\text{Max}} \quad C_i = f(q_1, \dots, q_i) \\
 & \text{s.t.} \\
 & 0 \leq q_i \leq w_i \quad , \\
 & \sum_{j=1}^n q_{ij} = Q_{Ti} \\
 & q_k = q_k^* \quad (k = 1, \dots, i-1)
 \end{aligned} \tag{3.1}$$

where C_i is the PCE concentration in the WTP at stress period i (ML^{-3}); n is the number of active water-supply wells in stress period i ; q_i is an n -dimensional vector of pumping rates at stress period i (L^3T^{-1}); w_i is an n -dimensional vector of the upper bound of q_i at

stress period i (pumping capacities) (L^3T^{-1}); Q_{Ti} is the total water demand at stress period i (L^3T^{-1}); and q_k^* is the optimal pumping schedule for stress period k (L^3T^{-1}).

In the optimization problem given in Equation (3.1), q_1, \dots, q_{i-1} are known, and C_i is only a function of q_i . Thus, to obtain the maximum PCE concentration C_i , only the pumping schedule of stress period i needs to be optimized based on the optimal pumping schedules of the previous stress periods. By formulating the problem in this way, the dimensions of the problem are reduced significantly, and the computational demand becomes manageable.

The optimization model for the minimum PCE concentration in the WTP is similar:

$$\begin{aligned} \underset{q_i \in R^n}{Min} \quad & C_i = f(q_1, \dots, q_i) \\ \text{s.t.} \quad & \\ & 0 \leq q_i \leq w_i \\ & \sum_{j=1}^n q_{ij} = Q_{Ti} \\ & q_k = q_k^* \quad (k = 1, \dots, i-1) \end{aligned} \quad (3.2)$$

The explanations used for this equation is the same as given for Equation (3.1).

Problem (3.2) can be easily solved by using the same method as used in the solution of the optimization problem given in Equation (3.1), because it can be re-written as:

$$\begin{aligned} \underset{q_i \in R^n}{Max} \quad & C_i' = -C_i = -f(q_1, \dots, q_i) \\ \text{s.t.} \quad & \\ & 0 \leq q_i \leq w_i \\ & \sum_{j=1}^n q_{ij} = Q_{Ti} \\ & q_k = q_k^* \quad (k = 1, \dots, i-1) \end{aligned} \quad (3.3)$$

Therefore, in this report only the “maximization” problem given in Equation (3.1) is used as an example when describing the optimization method.

3.2 Selection of the optimization method

For optimization problems given in Equations (3.1) and (3.2), the PCE concentration in the WTP is calculated by using the following governing equations:

$$\frac{\partial}{\partial x} (K_{xx} \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y} (K_{yy} \frac{\partial h}{\partial y}) + \frac{\partial}{\partial z} (K_{zz} \frac{\partial h}{\partial z}) + W = S_s \frac{\partial h}{\partial t}; \quad (3.4)$$

$$\frac{\partial(\theta C^k)}{\partial t} = \frac{\partial}{\partial x_i} (\theta D_{ij} \frac{\partial C^k}{\partial x_j}) - \frac{\partial}{\partial x_i} (\theta v_i C^k) + q_s C_s^k + \sum R_n; \quad (3.5)$$

and,

$$C_i = \frac{\sum_{j=1}^n q_{ij} c_{ij}}{Q_{Ti}}. \quad (3.6)$$

For the definition of the terms used in these equations, please refer to the text following Equations (2.1), (2.2), and (2.3). Among Equations (3.4), (3.5), and (3.6), Equation (3.4) is used in MODFLOW simulation for obtaining piezometric head distribution and groundwater flow velocity between adjacent nodes; Equation (3.5) is used in MT3DMS simulation to obtain the PCE concentration distribution; and Equation (3.6) is used to calculate the PCE concentration in the WTP.

A study of these three equations shows that optimization problems given in Equations (3.1) and (3.2) are multidimensional nonlinear optimization problems with linear constraints, which are much harder to solve and more computationally intensive than the linear optimization problems. Moreover, the objective functions are nonconcave or nonconvex, which imposes more difficulty in finding a global optimal solution. Significant literature exists on optimization methods for the solution of nonlinear optimization problems. Some of these methods are introduced briefly in the following sections.

3.2.1 The Downhill Simplex method

The Downhill Simplex method is an optimization method for multidimensional nonlinear problems that does not require evaluating the derivative of the objective function but uses only the objective function values [Press et al., 1989]. For an N-dimensional minimization problem, the Downhill Simplex Method starts with $N+1$ initial points (feasible solutions), which define an initial simplex, and then moves step by step towards the optimal solution. Each step is called a reflection. For a minimization problem, in each reflection the point of the simplex which has the largest value is found and moved through the opposite face of the simplex to a lower point, until the solution meets the termination criterion. In the Downhill Simplex method, although derivatives are not required, this approach is still not quite efficient considering the number of objective function evaluations it requires.

3.2.2 The Steepest Descent method

The Steepest Descent method is a non-linear optimization method that uses the derivative information of the objective function [Press et al., 1989]. To solve a minimization problem by using this method, starting from an initial point, the downhill gradient at that point is calculated, and a minimization point along the gradient direction is found. From that point, the downhill gradient is calculated, and another point along the gradient direction is found. By following this gradient direction on the objective function, an optimal solution that meets termination criterion can be found.

The problem with the Steepest Gradient method is that the iterated solutions may move

in a direction of reversed gradient paths because the gradient at a new point can be perpendicular to the previous gradient. This increases the computational burden and may lead to an inefficient method. Another problem for this method is that often the solution will be trapped in a local optimal solution.

3.2.3 The Conjugate Gradient method

Similar to the Steepest Descent method, the Conjugate Gradient method uses the derivative information to find the optimal solution for a non-linear optimization problem [Press et al., 1989]. This method differs from the Steepest Descent method in the following sense. The Conjugate Gradient method is improved in such a way that, for each movement towards the solution, the direction of movement is constructed to be conjugate to the old gradient. By doing this, an optimal solution can be achieved more efficiently.

Even though the Conjugate Gradient method is more efficient than Steepest Descent method, the calculation of derivatives of the objective function at each iteration step is still a heavy computational burden. Also similar to the Steepest Decent method, the possibility for the solution of the Conjugate Gradient method to be a local optimum instead of a global optimum is very high.

3.2.4 Genetic Algorithms

Genetic Algorithms (GA) get their name since the computational steps used are based on the evolutionary process observed in nature [Chinneck, 2006]. Their application requires the solution to be expressed as a string. Using a population of strings, an objective function value can be calculated for each string for its “fitness” evaluation.

During a GA process, first an initial population is generated and the fitness of each string is evaluated. Then, a mating pool is generated from the current population using several GA operations. For example, crossover operation (two parent strings obtained from the mating pool exchange part of their strings to form two new child strings) and mutation operation (values at some points of some strings are changed randomly) are applied to generate the new population. After the generation of new population, the fitness of each new string is evaluated again. This evolutionary process leads to the most fit strings to remain and accumulate in the population. If the termination criterion is met, the process is stopped. Otherwise, the process will start again based on the new generation of population.

A good aspect of GA is that the process can yield better and better solutions without reliance on gradients. Another advantage of GA is that they search the optimal solution globally and, thus the solution is sometimes better than those obtained from other methods mentioned previously. However, considering the computation power required for the evaluation of fitness of each string, if the computation time of the simulation tools required to solve the problem is large and if the mating pool is also large, then GA can be

more computationally demanding than the other methods discussed earlier.

Based on the review given above one can conclude that, for a complex nonlinear optimization problem, any of the methods discussed above can be computationally quite demanding. To reduce computational demand, a new optimization method identified as “rank-and-assign” method, which will be introduced in detail in the next section, has been developed uniquely for the problem discussed in this study. The few cases that can not be solved by the rank-and-assign method are optimized by the improved gradient method.

3.3 Introduction to PSOpS

Based on the two optimization techniques (rank-and-assign and improved Conjugate gradient methods) and simulation models (MODFLOW and MT3DMS), a procedure identified as PSOpS (Pumping Schedule Optimization system) has been developed to optimize the pumping schedule for the “earliest” or the “latest” PCE arrival time at the Tarawa Terrace WTP using the simulation/optimization approach. In PSOpS, MODFLOW and MT3DMS are used to simulate the groundwater flow and contaminant fate-and-transport conditions for the derivative calculations that are necessary in the solution of the optimization problem, and the optimization techniques are used within the same procedure to optimize the pumping schedules.

3.3.1 Methodology of PSOpS

The pumping schedule adjustment necessary to achieve the maximum PCE concentration level in the WTP, which is analogous to the earliest arrival time solution we are seeking, is solved by the procedure described in Figure 3.1. The variables and abbreviations used in Figure 3.1 are defined as follows:

Q_{Ti} : total pumping demand for the stress period i ;

$C_i^{(k)}$: PCE concentration in the WTP in the stress period i after the k^{th} iteration;

q_{ij} : the pumping rate of the water-supply well j at the stress period i ;

$(\frac{\partial C_i}{\partial q_{ij}})^{(k)}$: the change of PCE concentration in the WTP for the stress period i caused by the unit change of q_{ij} after the k^{th} iteration;

$q_i^{(k)}$: the pumping schedule vector for the stress period i after the k^{th} iteration which consists of q_{ij} of all water-supply wells at the stress period i ;

$\nabla C_i(q_i^{(k)})$: the concentration gradient vector for $q_i^{(k)}$ which consists of $(\frac{\partial C_i}{\partial q_{ij}})^{(k)}$ of all active water-supply wells at the stress period i ;

$\|\nabla C_i(q_i^{(k)})\|$: the norm of $\nabla C_i(q_i^{(k)})$, which is the maximum absolute value of $(\frac{\partial C_i}{\partial q_{ij}})^{(k)}$;

w_i : pumping capacity vector for the stress period i ;

$SQ_i^{(k)}$: the sequence of $(\frac{\partial C_i}{\partial q_{ij}})^{(k)}$; and,

ε : a pre-defined termination criterion. If $\|\nabla C_i(q_i^{(k)})\|$ is less than ε , the pumping schedule of the stress period i is considered to be optimal.

The assumptions made in PSOpS are as follows:

- i. When $\|\nabla C_i(q_i^{(k)})\|$ is less than ε , the pumping schedule for the current stress period i is optimal, and no further update is required;
- ii. The total pumping rate of all water-supply wells at stress period i is equal to the total pumping demand of that stress period;
- iii. Pumping rate in a water-supply well is always less than or equal to its pumping capacity; and,
- iv. Water-supply wells outside of the simulated region (well 6, well 7, and well TT-45 in this case) are considered as one well with zero $\frac{\partial C_i}{\partial u_{ij}}$ value. In other words, the pumping rates in these wells can be adjusted but they do not provide contaminant mass into the WTP.

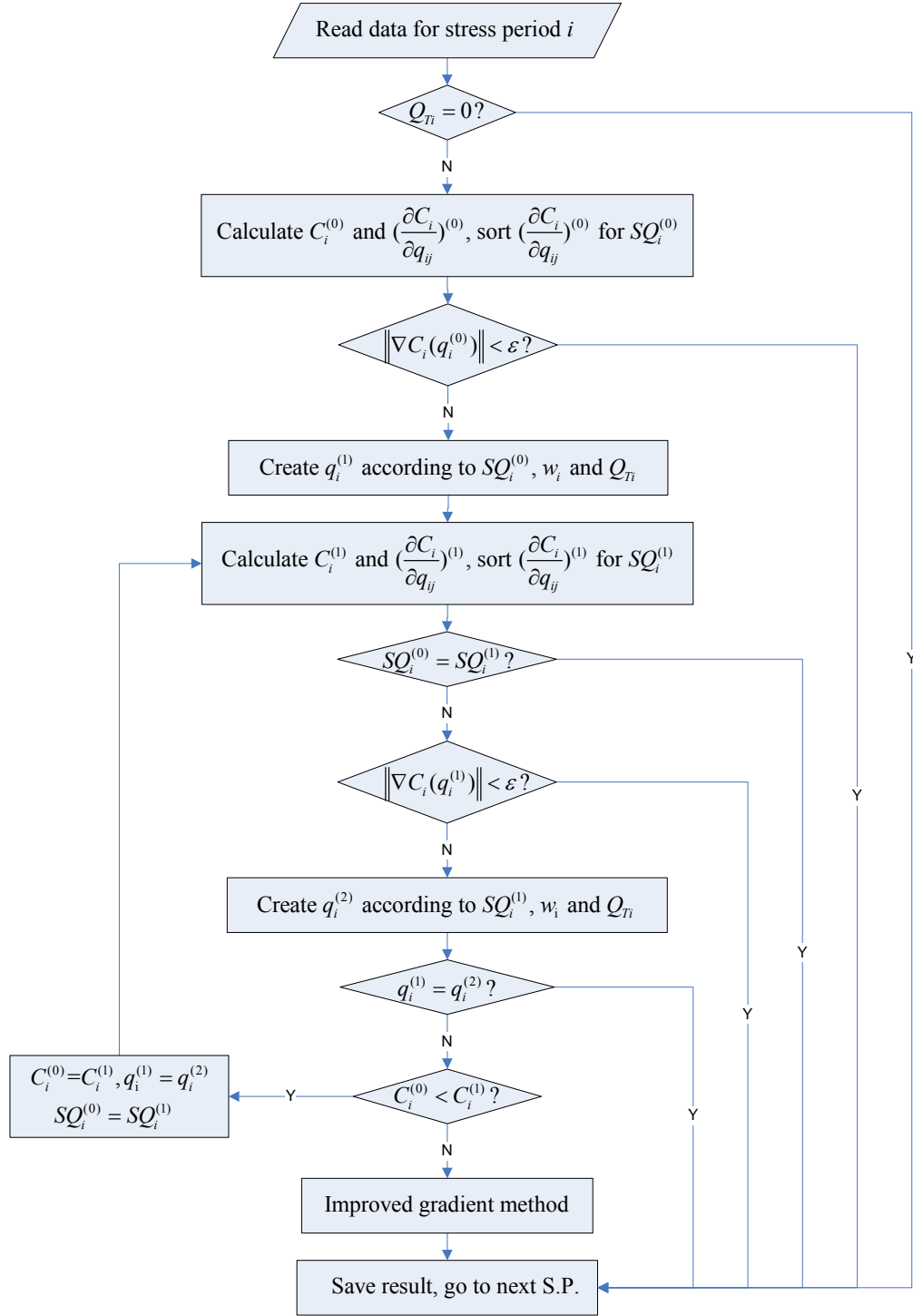


Figure 3.1. Flowchart for PSOpS

Following the procedure given in Figure 3.1, PSOpS optimizes the pumping schedules for maximum PCE concentration levels in the WTP at stress period i as outlined in the step-by-step process given below:

- i. Read input data for the stress period i , such as the total pumping demand (Q_{Ti}), the pumping capacities (w_i), and the initial pumping schedule ($q_i^{(0)}$);
- ii. If Q_{Ti} is equal to zero, no pumping schedule update is required, go to step (xiii); otherwise go to step (iii);
- iii. Run MODFLOW and MT3DMS for stress period i to obtain $C_i^{(0)}$, then run MODFLOW and MT3DMS for another n times, where n is the number of active wells in the stress period i , with a unit change in pumping rate to calculate the gradients $(\frac{\partial C_i}{\partial q_{ij}})^{(0)}$ for each active well. After this computation, sort the $(\frac{\partial C_i}{\partial q_{ij}})^{(0)}$ values for $SQ_i^{(0)}$;
- iv. If $\|\nabla C_i(q_i^{(0)})\|$ is less than ε , no update for the stress period i is required, then go to step (xiii); otherwise go to step (v);
- v. Update the pumping schedule of stress period i to $q_i^{(1)}$ using “rank-and-assign” method according to $SQ_i^{(0)}$, w_i , and Q_{Ti} (please refer to section 3.3.2 for a detailed information on these variables);
- vi. Similar to step (iii), update $C_i^{(1)}$ using $q_i^{(1)}$, calculate $(\frac{\partial C_i}{\partial q_{ij}})^{(1)}$ values and sort these values to obtain $SQ_i^{(1)}$;
- vii. Compare $SQ_i^{(0)}$ and $SQ_i^{(1)}$. If they are the same, $q_i^{(1)}$ is the optimal pumping schedule for the stress period i , then go to step (xiii); otherwise go to step (viii);
- viii. If $\|\nabla C_i(q_i^{(1)})\|$ is less than ε , $q_i^{(1)}$ is the optimum, then go to step (xiii); otherwise go to step (ix);
- ix. Similar to step (v), update $q_i^{(1)}$ to $q_i^{(2)}$ using the “rank-and-assign” method according to $SQ_i^{(1)}$, w_i , and Q_{Ti} ;
- x. Compare $q_i^{(1)}$ and $q_i^{(2)}$. If they are the same, then go to step (xiii); otherwise go to step (xi);
- xi. Compare $C_i^{(0)}$ and $C_i^{(1)}$. If $C_i^{(0)}$ is less than $C_i^{(1)}$, use $C_i^{(1)}$, $SQ_i^{(1)}$, and $q_i^{(2)}$ to replace $C_i^{(0)}$, $SQ_i^{(0)}$, and $q_i^{(1)}$, then go to step (vi) and update again; otherwise

- go to step (xii);
- xii. Optimize $q_i^{(2)}$ using the improved gradient method (please refer to 3.3.3 for detailed information);
 - xiii. Run MODFLOW and MT3DMS simulations using the optimal pumping schedule for the stress period i again, and save piezometric head and concentration distribution information at the end of the stress period i for optimization of pumping schedule of the next stress period.

Optimization of the pumping schedule to obtain the minimum PCE concentration in the WTP is equivalent to the optimization of the pumping schedule for the maximum PCE concentration in the WTP with the objective function multiplied by minus one, and therefore will not be discussed here.

3.3.2 The rank-and-assign method

The rank-and-assign method was specially developed for PSOpS. This method updates the pumping schedule for maximum or minimum contaminant concentration levels in the WTP based on the derivative, pumping capacity, and the total pumping demand information available for the system. The name of this method reflects the steps it follows to update the pumping schedule – it first “ranks” the gradients, and then “assigns” the pumping rates to each water-supply well according to this ranking.

Steps (iii) to step (xi) shown in Figure 3.1 describe the rank-and-assign optimization technique. In step (v), by assuming an $SQ_i^{(0)}$ with the following ranking,

$$\left(\frac{\partial C_i}{\partial q_{i1}}\right)^{(0)} \geq \dots \geq \left(\frac{\partial C_i}{\partial q_{ik}}\right)^{(0)} \geq \dots \geq \left(\frac{\partial C_i}{\partial q_{in}}\right)^{(0)}, \quad (3.7)$$

the procedure below is followed to assign the $q_i^{(1)}$ to yield the maximum PCE concentration in the WTP:

- i. Assign the pumping capacity of the first well in $SQ_i^{(0)}$ as its pumping rate. If the total pumping demand is less than the pumping capacity of that well, assign the total pumping demand as its pumping rate, and go to step (iv);
- ii. If the remaining pumping demand is greater than the pumping capacity of the next well in $SQ_i^{(0)}$, assign the pumping capacity of that well as its pumping rate, and repeat step (ii), otherwise go to step (iii);
- iii. Assign the remaining pumping demand as the pumping rate of the next well in $SQ_i^{(0)}$; and,
- iv. Assign zero pumping rates to all other wells that are left in the $SQ_i^{(0)}$ list.

In the rank-and-assign method, the optimized pumping schedule satisfying the condition “ $SQ_i^{(0)} = SQ_i^{(1)}$ ” is at least a local optimum because it satisfies the Kuhn-Tucker condition [Kuhn and Tucker, 1951]. The Kuhn-Tucker condition is described below.

Consider the problem:

$$\begin{aligned} & \underset{x \in R^n}{\text{Min}} f(x) \\ & \text{s.t.} \\ & g_i(x) \leq 0 \\ & h_j(x) = 0 \end{aligned} \quad (3.8)$$

where $g_i(x)$ ($i = 1, \dots, m$) is the non-equality constraints; $h_j(x)$ ($j = 1, \dots, l$) is the equality constraints; m is the number of non-equality constraints; and, l is the number of equality constraints.

Suppose that the objective function $f: R^n \rightarrow R$ and the constraint functions $g_i: R^n \rightarrow R$ and $h_j: R^n \rightarrow R$ are continuously differentiable at a point $x^* \in S$. If x^* is a local minimum, then constants $\lambda_i \geq 0$ ($i = 1, \dots, m$) and μ_j ($j = 1, \dots, l$) exist such that

$$\begin{aligned} \nabla f(x^*) + \sum_{i=1}^m \lambda_i \nabla g_i(x^*) + \sum_{j=1}^l \mu_j \nabla h_j(x^*) &= 0 \\ \lambda_i g_i(x^*) &= 0 \text{ for all } i = 1, \dots, m \end{aligned} \quad (3.9)$$

To prove that a solution from the “rank-and-assign” method satisfies the Kuhn-Tucker condition, the problem for one stress period is reformulated as:

$$\begin{aligned} & \underset{q \in R^n}{\text{Min}} -C = -f(q) \\ & \text{s.t.} \\ & -q_i \leq 0 \quad (i = 1, \dots, n) \\ & q_i - w_i \leq 0 \quad (i = 1, \dots, n) \\ & \sum_{i=1}^n q_i - Q_T = 0 \end{aligned} \quad (3.10)$$

where C is the PCE concentration in the WTP; n is the number of active water-supply wells; q is an n -dimensional vector of pumping rates; q_i is the pumping rate of well i ; w_i is the pumping capacity for well i ; and, Q_T is the total water demand.

The Kuhn-Tucker conditions for the problem given in Equation (3.10) are,

$$\begin{aligned}
-\frac{\partial f}{\partial q_i} - \lambda_i + \omega_i + \mu &= 0 \quad (i = 1, \dots, n) \\
\lambda_i q_i &= 0 \quad (i = 1, \dots, n) \\
\omega_i (q_i - w_i) &= 0 \quad (i = 1, \dots, n) \\
\lambda_i &\geq 0 \quad (i = 1, \dots, n) \\
\omega_i &\geq 0 \quad (i = 1, \dots, n)
\end{aligned} \tag{3.11}$$

Suppose the optimal solution from the rank-and-assign method is

$$q_i \begin{cases} = w_i & (i = 1, \dots, k-1) \\ \leq w_i & (i = k) \\ = 0 & (i = k+1, \dots, n) \end{cases}, \tag{3.12}$$

while the following condition is satisfied,

$$\frac{\partial f}{\partial q_1} \geq \dots \geq \frac{\partial f}{\partial q_k} \geq \dots \geq \frac{\partial f}{\partial q_n}. \tag{3.13}$$

For $i \leq k$, since $q_i > 0$, to satisfy $\lambda_i q_i = 0$, there is:

$$\lambda_i = 0 \quad (i = 1, \dots, k). \tag{3.14}$$

According to equation: $-\frac{\partial f}{\partial q_i} - \lambda_i + \omega_i + \mu = 0$, there is:

$$\omega_i = \frac{\partial f}{\partial q_i} - \mu \quad (i = 1, \dots, k). \tag{3.15}$$

Let $\mu = \frac{\partial f}{\partial q_k}$, there is:

$$\omega_k = 0. \tag{3.16}$$

Since $\frac{\partial f}{\partial q_i} \geq \frac{\partial f}{\partial q_k}$ for $i < k$, there is:

$$\omega_i = \frac{\partial f}{\partial q_i} - \frac{\partial f}{\partial q_k} \geq 0 \quad (i = 1, \dots, k-1). \tag{3.17}$$

For $i > k$, since $q_i = 0$, to satisfy $\omega_i (q_i - w_i) = 0$, there must be:

$$\omega_i = 0 \quad (i = k+1, \dots, n). \tag{3.18}$$

According to equation $-\frac{\partial f}{\partial q_i} - \lambda_i + \omega_i + \mu = 0$ there is:

$$\lambda_i = \mu - \frac{\partial f}{\partial q_i} = \frac{\partial f}{\partial q_k} - \frac{\partial f}{\partial q_i} \quad (i = k+1, \dots, n). \quad (3.19)$$

Since $\frac{\partial f}{\partial q_k} \geq \frac{\partial f}{\partial q_i}$ for $i > k$, it is known that,

$$\lambda_i = \frac{\partial f}{\partial q_k} - \frac{\partial f}{\partial q_i} \geq 0 \quad (i = k+1, \dots, n) \quad (3.20)$$

Therefore, the Kuhn-Tucker conditions are satisfied.

The Kuhn-Tucker conditions are the necessary conditions for a solution to be optimal. For an optimization problem with convex (minimization problem) or concave (maximization problem) objective function, the Kuhn-Tucker conditions are also sufficient conditions for the solution to be a global optimum. However, since the objective function in this problem is nonconvex (or nonconcave), the solution obtained from the rank-and-assign method is not guaranteed to be the global optimum, which is same as the situation associated with many other nonlinear optimization methods. In this sense, the rank-and-assign method trades computational efficiency with global optimality.

3.3.3 The improved gradient method

As shown in Figure 3.1, in PSOpS application, the rank-and-assign method is applied first to each stress period. If the optimal solution can not be obtained from the rank-and-assign optimization process, an improved gradient method is used for the optimal solution. The improved gradient method is similar to the steepest descent method introduced previously. In PSOpS, the steepest descent method is further improved from two aspects: (1) reducing the dimension of the optimization problem and, (2) projecting the gradient to satisfy the equality constraint.

In the improved gradient method, the ranking of active pumping wells in $SQ_i^{(0)}$ and $SQ_i^{(1)}$ obtained from the rank-and-assign method are compared, and wells with same rankings in both sequences are exempted from the optimization process. Thus, the dimension of the optimization problem can be reduced significantly along with the computational cost. For example, assuming that there are five pumping wells with $SQ_i^{(0)}$ and $SQ_i^{(1)}$ as,

$$SQ_i^{(0)} : \left(\frac{\partial C_i}{\partial q_{i1}}\right)^{(0)} \geq \left(\frac{\partial C_i}{\partial q_{i2}}\right)^{(0)} \geq \left(\frac{\partial C_i}{\partial q_{i3}}\right)^{(0)} \geq \left(\frac{\partial C_i}{\partial q_{i4}}\right)^{(0)} \geq \left(\frac{\partial C_i}{\partial q_{i5}}\right)^{(0)}; \quad (3.21)$$

$$SQ_i^{(1)} : \left(\frac{\partial C_i}{\partial q_{i1}}\right)^{(1)} \geq \left(\frac{\partial C_i}{\partial q_{i4}}\right)^{(1)} \geq \left(\frac{\partial C_i}{\partial q_{i2}}\right)^{(1)} \geq \left(\frac{\partial C_i}{\partial q_{i3}}\right)^{(1)} \geq \left(\frac{\partial C_i}{\partial q_{i5}}\right)^{(1)}. \quad (3.22)$$

Between the two sequences given above, only wells 2, 3, and 4 have different rankings. Therefore, in the improved gradient method, only wells 2, 3, and 4 are considered as variables for optimization, and the dimension of the problem is reduced from 5 to 3, accordingly.

This variable-elimination step is logical. Using the maximization process as an example, after $SQ_i^{(0)}$ is obtained the pumping schedule would be updated according to the procedure described in the rank-and-assign method. Then, according to Equation (3.22), $SQ_i^{(1)}$ indicates that well 1 still has the most potential to increase the contaminant concentration by increasing its pumping rate. However, the pumping rate in well 1 has reached its pumping capacity and can not be increased any further. Therefore, it is exempted from optimization. The case for well 5 is similar—to increase the contaminant concentration its pumping rate is supposed to be decreased, while its pumping rate is already zero. (If the pumping rate of well 5 is not zero, then according to the description of the “rank-and-assign” method we know that the pumping rates of wells 2, 3, and 4 are at their pumping capacities, respectively, and the pumping schedule can not be updated any more.)

After eliminating water-supply wells with same rankings in both sequences, the gradient of the remaining wells is then projected to the feasible solution space by subtracting the same amount from all the derivatives to make the summation of the resulting derivatives to be zero. The equality constraint of the optimization problem can be eliminated by applying this gradient projection because the process guarantees the summation of the resulting pumping rates to be constant.

The improved gradient method works through the steps shown in Figure 3.2. Some variables are the same as defined for Figure 3.1, the others are defined below.

$d^{(k)}$: The search direction of the optimal solution for the k^{th} iteration. Its dimension is the same as the dimension of the pumping rate vector.

λ_k : The step size of the solution increment for the k^{th} iteration.

$\nabla^* C_i(q_i^{(k)})$: The projection of $\nabla C_i(q_i^{(k)})$ in the feasible solution space.

Computational steps of the improved gradient method in obtaining the maximum PCE concentration levels at the WTP at stress period i are:

- i. Eliminate the decision variables with the same rankings in $SQ_i^{(0)}$ and $SQ_i^{(1)}$;
- ii. Set $d^{(1)}$ to be equal to $\nabla^* C_i(q_i^{(1)})$;

- iii. Find λ_k to maximize $C_i(q_i^{(k)} + \lambda d^{(k)})$ using the one-dimensional line search method;
- iv. Update $q_i^{(k)}$ to $q_i^{(k+1)}$;
- v. If $\|\nabla^* C_i(q_i^{(k+1)})\|$ is less than ε , $q_i^{(k+1)}$ is the optimum, then go to step (vii); otherwise go to the next step;
- vi. Update $d^{(k)}$ to $d^{(k+1)}$, go to step (iii) for another iteration; and
- vii. Save the optimal solution.

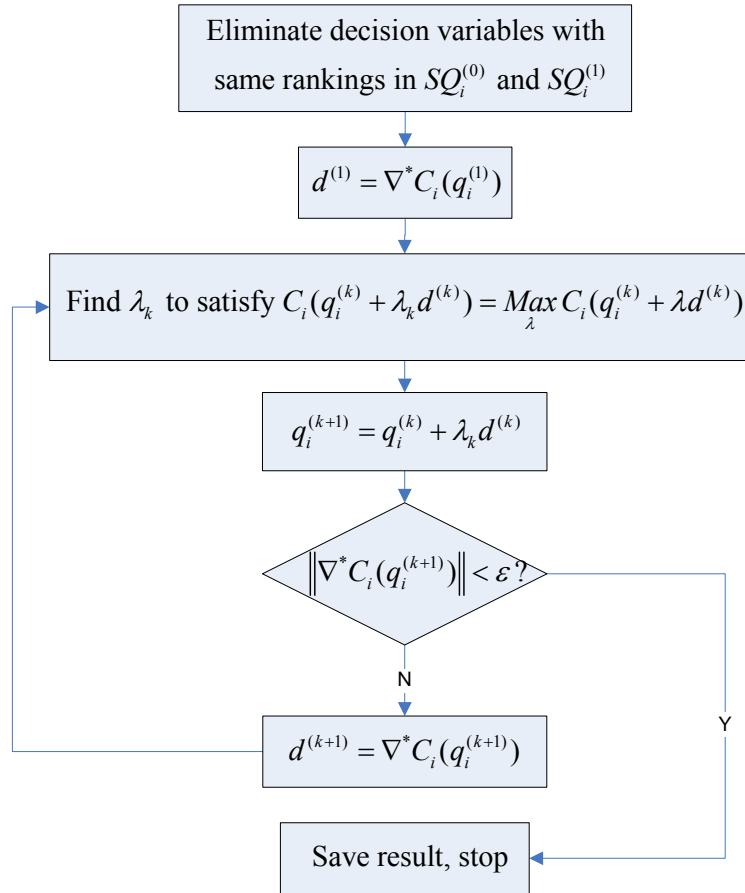


Figure 3.2. Flowchart for the improved gradient method

3.3.4 Improvement of computational efficiency

The goal of the development of PSOpS is to improve the computational efficiency and this has been achieved as follows.

- i. ***The reduction of the dimensions of the problem:*** By reformulating the problem, only the pumping schedule of the current stress period needs to be updated to obtain the optimal contaminant concentration in the WTP. A problem that can not

- be solved by the rank-and-assign technique and can be solved by the improved Conjugate Gradient method which further reduces the dimension of the problem;
- ii. **The reduction of the number of iterations for the optimization:** Simulation results of this study indicate that most “rank-and-assign” optimizations converge within two iterations; and,
- iii. **Elimination of repeated simulations:** At the end of optimization for each stress period, the piezometric head and concentration distributions are updated and saved as the starting point of the optimization of the next stress period.

By applying PSOpS, an optimal pumping schedule for the problem can be obtained within four to five days on a desktop workstation with 2 GHz CPU and 1 GB memory. A summary of the optimization status for the maximum PCE concentration levels in the WTP is given in Table 3.1. In 106 of 528 stress periods, no water was supplied to the WTP (January 1951 – December 1951 and March 1987 – December 1994). Among the remaining 422 stress periods, the pumping schedules in 417 stress periods were updated by the rank-and-assign method, which accounts for 98.8% of the solution. This percentage indicates that the rank-and-assign method works efficiently for this problem.

Table 3.1. Summary of the optimization status for the maximum PCE concentration

Optimization status	Number of cases	Percentage
$\ \nabla C_i(q_i^{(0)})\ < \varepsilon$, no update	3	0.6
$SQ_i^{(0)} = SQ_i^{(1)}$	369	69.9
$\ \nabla C_i(q_i^{(1)})\ < \varepsilon$, no second update	7	1.3
$q_i^{(1)} = q_i^{(2)}$	41	7.8
Optimization using improved gradient method	2	0.4
No pumping and no update	106	20.0
Total	528	100

3.3.5 Input data for PSOpS

As introduced before, PSOpS was developed based on the simulation/optimization (S/O) approach. In PSOpS the groundwater simulation model MODFLOW and the contaminant fate-and-transport model MT3DMS are used as the simulators. Therefore, the original input files of MODFLOW and MT3DMS obtained from the ATSDR study can be used as input for PSOpS directly. Other than these files, only three files are required to provide simulation type, pumping capacities, and total pumping demand information as given below.

- i. **File type:** INFO
File contents: optimization type (“1” for maximization of the contaminant

- concentration and “2” for minimization of the contaminant concentration);
- ii. ***File type:*** PCP
File contents: Pumping capacities of each water-supply well at each stress period;
- iii. ***File type:*** TPD
File contents: Total pumping demand for each stress period.

Direct application of input files for MODFLOW and MT3DMS as input for PSOpS makes the generation of input files very efficient and convenient.

4 Simulation Results and Discussion

In this study, PSOpS was run three times: (i) the first run was to obtain the “early” PCE arrival time in the Tarawa Terrace WTP; (ii) the second run was to obtain the “late” PCE arrival time in the WTP; and, (iii) the third run was also to obtain the “late” PCE arrival time with a restriction that the pumping rate in well TT-26 was not to be assigned less than 25% of its pumping capacity. In all PSOpS applications the pumping rates in the water-supply wells are considered to be the only unknown variables. In this report, the optimal pumping schedules obtained from the three PSOpS runs are identified as the “Maximum Schedule” (Max. Sche.); the “Minimum Schedule I” (Min. Sche. I); and, the “Minimum Schedule II” (Min. Sche. II), respectively. The original pumping schedule obtained from the ATSDR study is identified as the “Original Schedule” (Org. Sche). In the following sections, results for these three optimized pumping schedules are discussed.

4.1 Optimization and simulation results for the Maximum Schedule

In the Maximum Schedule obtained from PSOpS the pumping rates of 419 stress periods are updated. Among them, the pumping rates from 417 stress periods are updated by the rank-and-assign method, which reduces the computational time significantly.

According to the ATSDR study, the water-supply wells in the Tarawa Terrace area started to pump in January 1952, while ABC One-Hour Cleaners started operations during January 1953. The output of PSOpS indicates that the first three-months of pumping in 1952 had negligible effect on the PCE concentration in the WTP after ABC One-Hour Cleaners started to release contaminants into the groundwater system. Except for those three stress periods, well TT-26 always pumped at its maximum pumping rates (pumping capacities) in the Maximum Schedule solution. This fact may be caused by the proximity of the location of well TT-26 to the ABC One-Hour Cleaners relative to the other wells (Figure 2.1) and its locating in the downstream groundwater flow direction relative to the location of ABC One-Hour Cleaners. A higher pumping rate in well TT-26 will generate a higher hydraulic gradient between the contaminant source and well TT-26. This would result in faster movement of contaminants from the source to well TT-26 and, thus, an early contaminant arrival time at the pumping well and the WTP. Pumping rates of well TT-26 under the Maximum Schedule are compared to its pumping capacities in Figure 4.1.

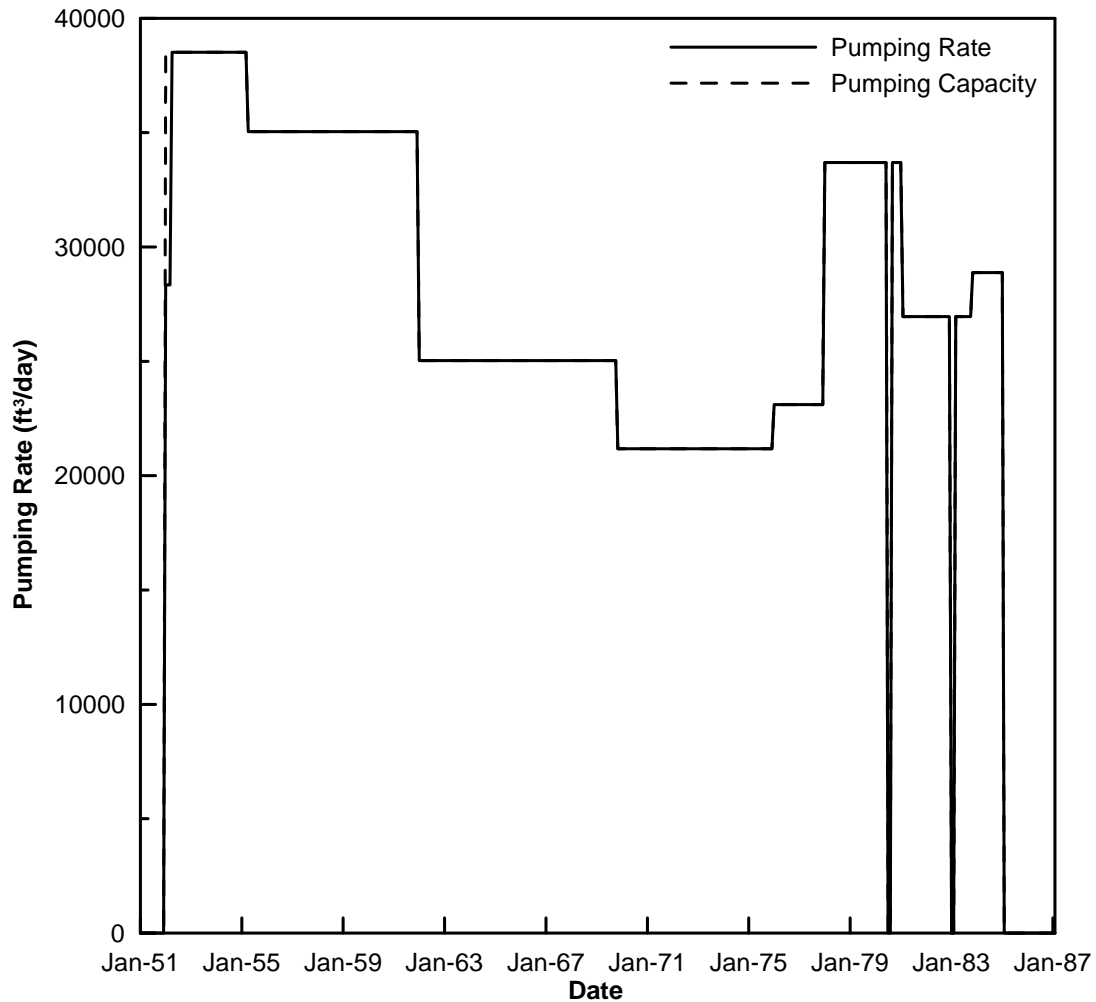


Figure 4.1. Pumping rate and pumping capacity of well TT-26 under the Maximum Schedule

4.1.1 PCE distribution in the groundwater system

While keeping the other input data unchanged, and using the Maximum Schedule as input for the WEL package, an MF2K simulation and an MT3DMS simulation were conducted to simulate the groundwater flow and PCE transport under the Maximum Schedule.

As expected, a variation in the pumping schedule changes the groundwater flow in the subsurface system, thus the PCE fate-and-transport in the aquifer domain also is changed. To illustrate this change, a comparison of the PCE distribution in the groundwater system of the Tarawa Terrace area and its vicinity under the Original Schedule and the Maximum Schedule are shown in Figures 4.2, 4.3 and 4.4. Only PCE distributions at stress periods 100, 200, 300, and 400 in layers 1, 3, and 5 are shown in these figures. The text at the bottom left corner of each illustration in these figures indicates the pumping schedule, the stress period, and the layer number. For example, “Org_SP100_L1” identifies a plot for PCE distribution in layer 1 at stress period 100 under the Original Schedule.

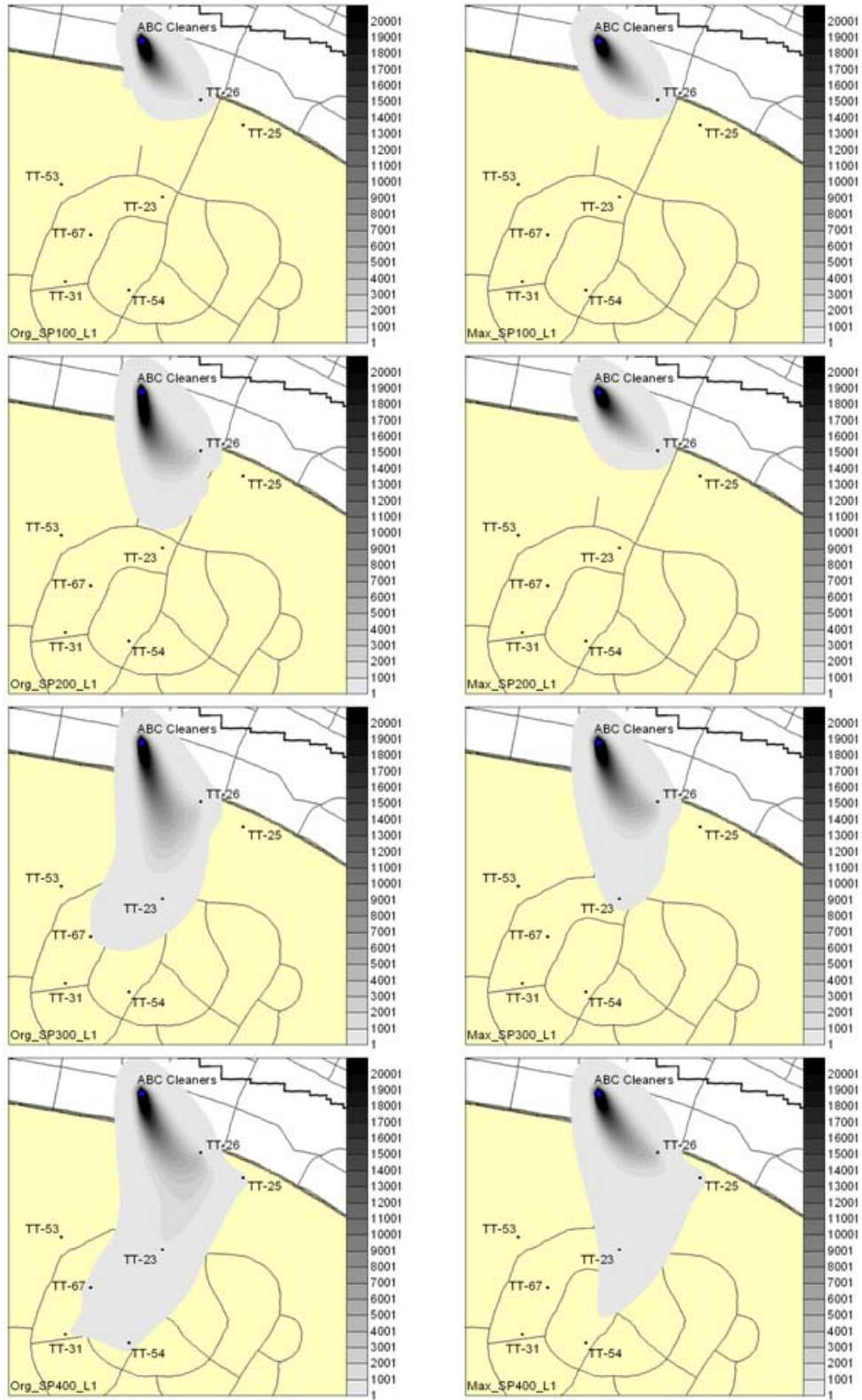


Figure 4.2. Comparison of PCE distribution in Layer 1 under the Original Schedule and the Maximum Schedule (Units: ppb)

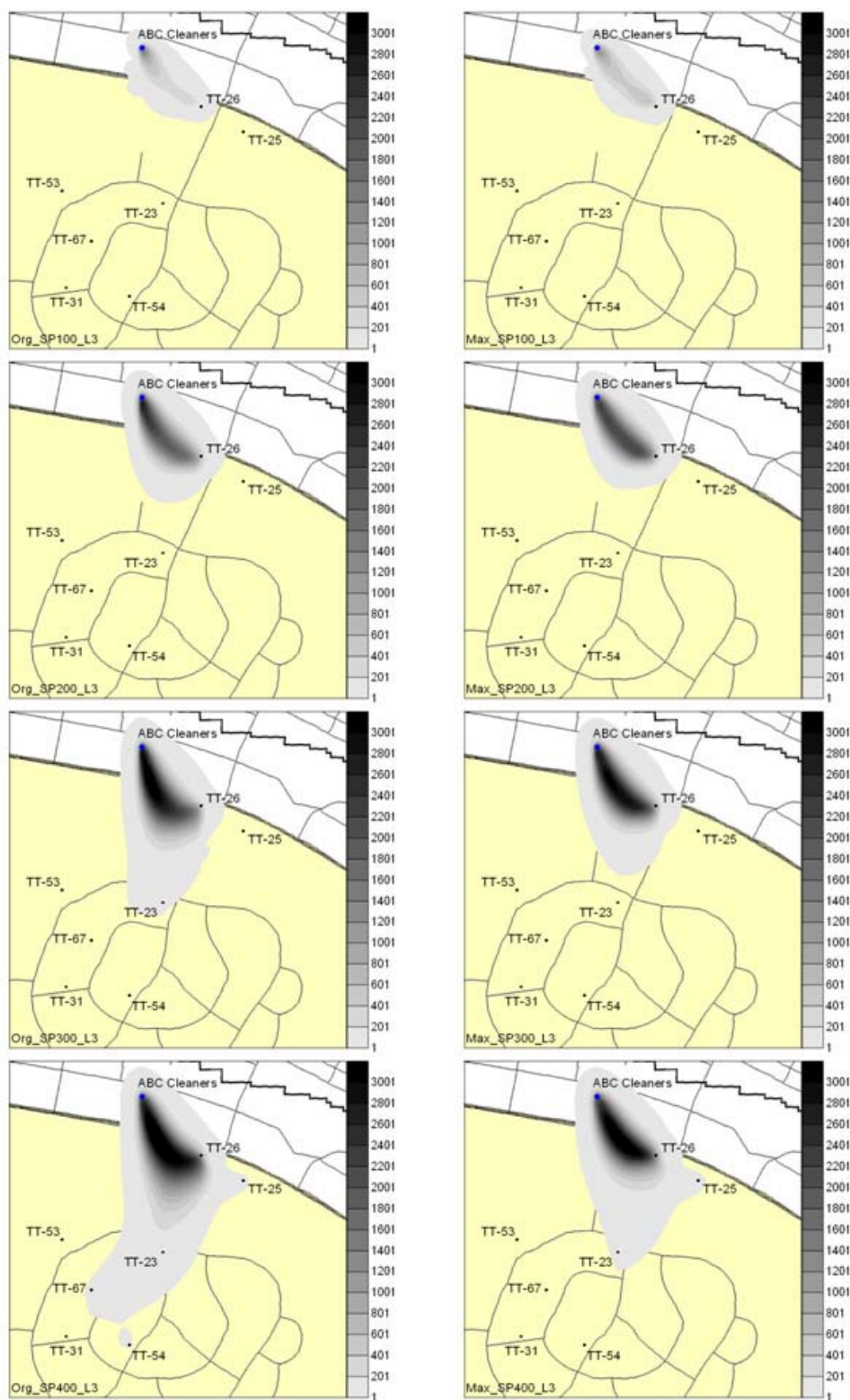


Figure 4.3. Comparison of PCE distribution in Layer 3 under the Original Schedule and the Maximum Schedule (Units: ppb)

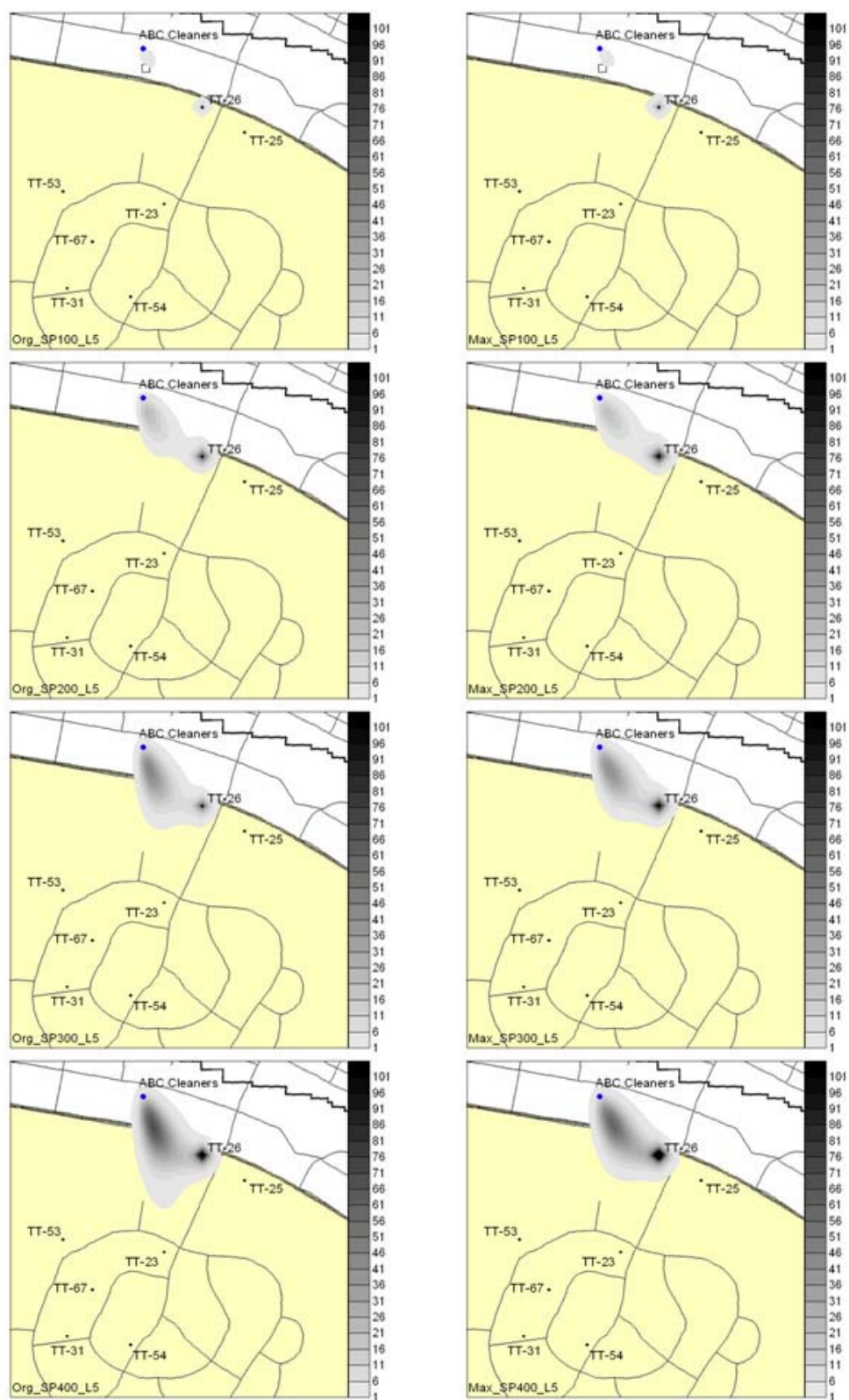


Figure 4.4. Comparison of PCE distribution in Layer 5 under the Original Schedule and the Maximum Schedule (Units: ppb)

The results given in Figures 4.2, 4.3, and 4.4 indicate that, when compared to the Original Schedule, the PCE contaminant plume under the Maximum Schedule is aggregated into a smaller domain and the front of the plume is directed more towards the location of well TT-26. This is because, under the Maximum Schedule, the higher pumping rate in well TT-26 creates a higher piezometric head gradient towards the location of well TT-26, which causes a faster groundwater flow towards and more contaminant mass entering into the well TT-26. Therefore, a higher PCE concentration in well TT-26 is expected under the Maximum Schedule.

4.1.2 PCE concentration in the water-supply wells

From the concentration observation file obtained from the MT3DMS simulation, the PCE concentration in water-supply wells is acquired. The results are compared to the PCE concentration distribution under the Original Schedule as shown in Figure 4.5.

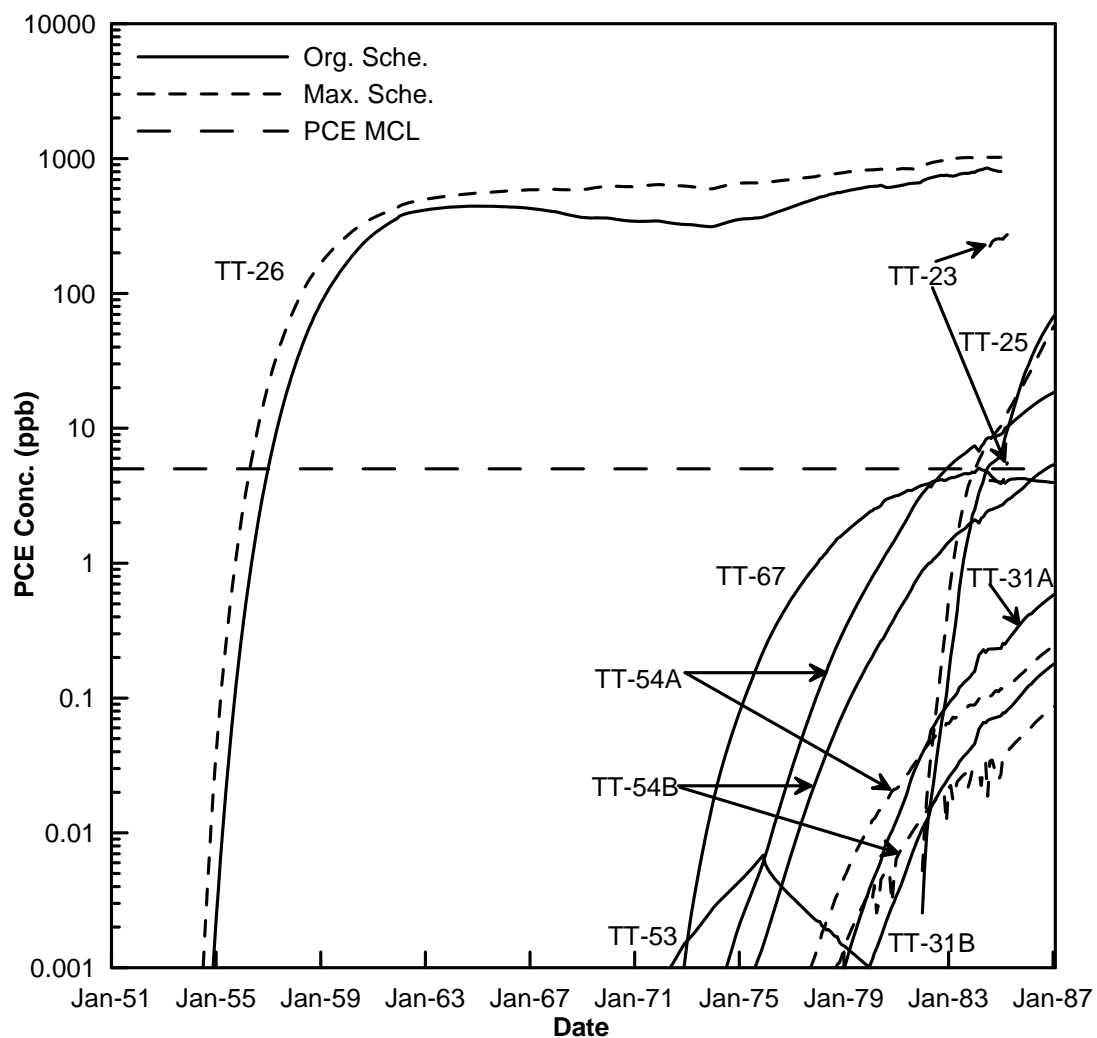


Figure 4.5. PCE concentrations in water-supply wells under the Original Schedule and the Maximum Schedule

The results presented in Figure 4.5 lead to the following observations for PCE concentrations in the water-supply wells under the Maximum Schedule:

- i. Instead of nine water-supply wells which had PCE concentrations higher than 0.001 ppb (well TT-26, TT-23, TT-25, TT-67, TT-54A, TT-54B, TT-31A, TT-31B, and TT-53) under the Original Schedule, under the Maximum Schedule there are only five pumping wells that had PCE concentrations higher than 0.001 ppb. These wells are TT-26, TT-23, TT-25, TT-54A, and TT-54B;
- ii. Throughout the simulation period, PCE concentrations in well TT-26 were always higher under the Maximum Schedule when compared to the concentrations obtained under the Original Schedule. More specifically, as shown in Figure 4.6, PCE concentrations in well TT-26 were much higher under the Maximum Schedule when compared with the Original Schedule results during the period of interest (1968 – 1985);
- iii. PCE concentration in well TT-25 was higher under the Maximum Schedule when compared with the Original Schedule results before October 1985 and was lower after that;
- iv. For well TT-23, TT-54A, and TT-54B, the PCE concentrations were lower under the Maximum Schedule when compared with the concentrations obtained under the Original Schedule;
- v. Under the Maximum Schedule, only three water-supply wells had PCE concentrations over 5 ppb. They are wells TT-26, TT-23, and TT-25. Among them, PCE concentration in well TT-26 was much higher than the MCL throughout the period of interest. The other two wells had PCE concentrations higher than the MCL only for a very short period of time;
- vi. PCE concentration in well TT-26 was much higher than those obtained in other wells throughout the simulation period. Since well TT-26 always pumped at its full capacity (except for the first three months of 1952), it was the major water-supply well that transported contaminants into the WTP under the Maximum Schedule.

Based on the observations given above, the difference of the PCE concentrations obtained in well TT-26 from different pumping schedules is further evaluated, and the following observations can be made:

- i. PCE concentration in well TT-26 reached 5 ppb in May 1956 under the Maximum Schedule, which was eight months earlier than the PCE MCL arrival time under the Original Schedule (January 1957). Since well TT-26 was the major contributor of PCE into the WTP, the PCE concentration in the WTP would also reach the MCL earlier under the Maximum Schedule;
- ii. PCE concentration in well TT-26 was much higher under the Maximum Schedule when compared to the concentration obtained under the Original Schedule during the period of interest. Between these two pumping schedules, the minimum difference of PCE concentration in well TT-26 is 169.62 ppb, the

maximum difference is 304.84 ppb and the average difference is 247.13 ppb (Table 4.1).

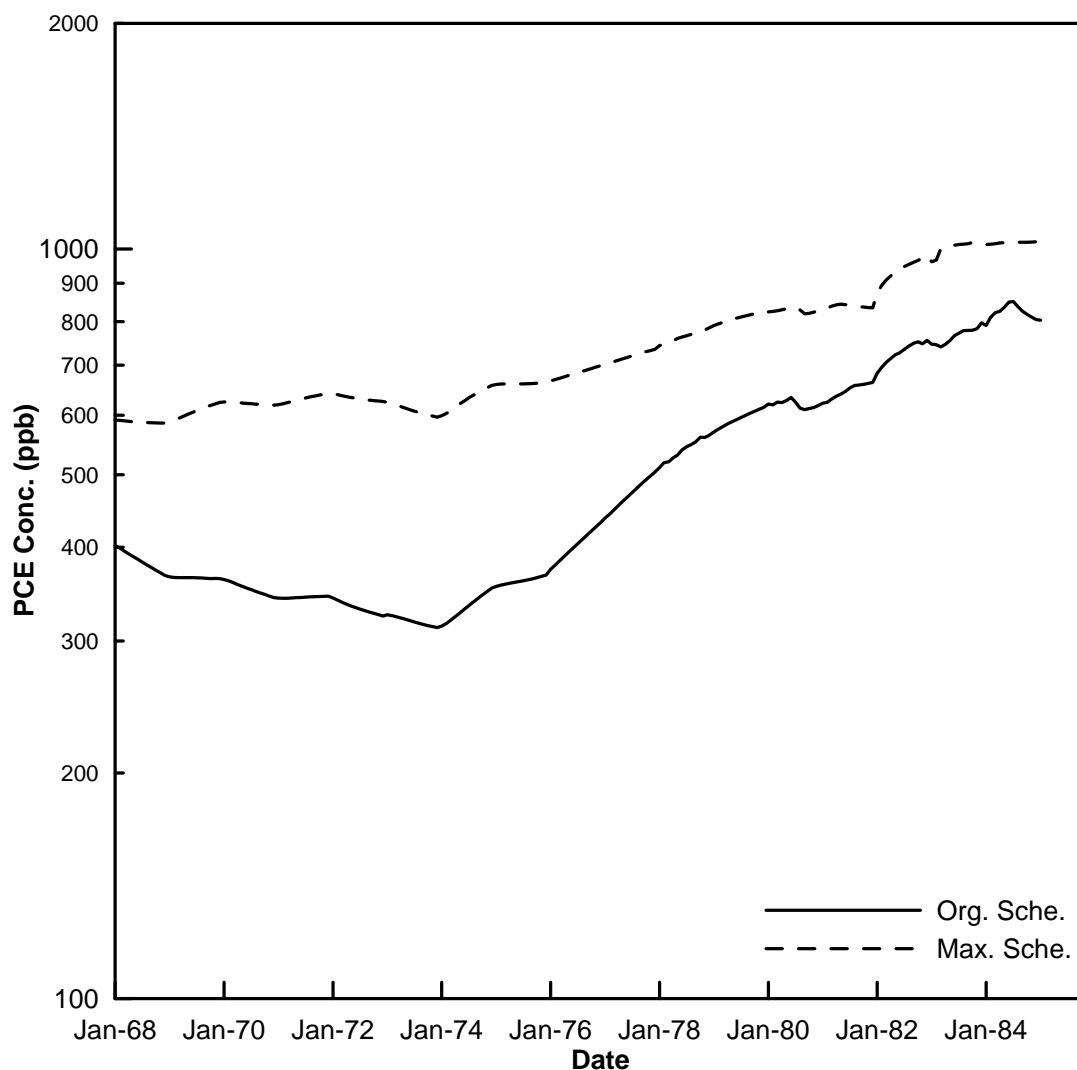


Figure 4.6. PCE concentrations in well TT-26 under the Original Schedule and the Maximum Schedule for period of interest

Table 4.1. PCE concentrations in well TT-26 under the Original Schedule and the Maximum Schedule for the period of interest* (Units: ppb)

	Maximum	Minimum	Average
Org. Sche.	312.62	851.19	494.36
Max. Sche.	585.98	1023.31	741.49
Difference	304.84	169.62	247.13

* Data for July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985 are not included.

4.1.3 PCE concentration in the WTP

Using the mixing model described in Equation (2.3), the PCE concentration in the Tarawa Terrace WTP under the Maximum Schedule was calculated and compared to that obtained under the Original Schedule. These comparisons are shown in Figures 4.7 and 4.8.

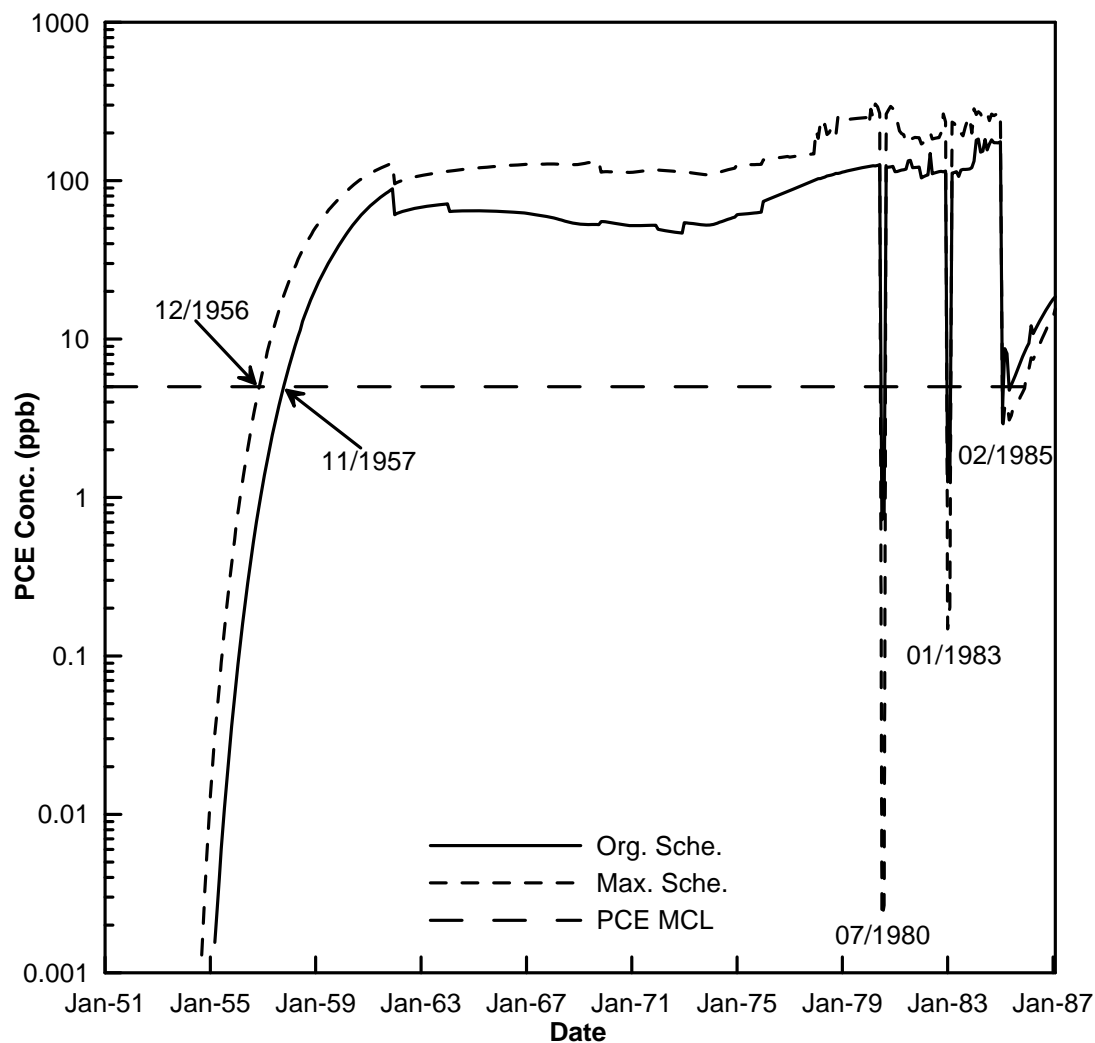


Figure 4.7. PCE concentrations in WTP under the Original Schedule and the Maximum Schedule

Results given in Figures 4.7 and 4.8 lead to the following observations:

- i. The PCE concentration in the WTP under the Maximum Schedule is significantly higher than that obtained from the Original Schedule except for the time period after February 1985, when well TT-26 was out of service. The higher PCE concentration in the WTP is caused by the higher pumping rate and the higher PCE concentration in well TT-26 under the Maximum Schedule;
- ii. The higher PCE concentration in the WTP is equivalent to the earlier

contaminant arrival time – the PCE concentration in the Tarawa Terrace WTP reached 5 ppb in December 1956, which is eleven months earlier than the Original Schedule (November 1957);

- iii. There are three sudden drops in PCE concentration in the WTP under the Maximum Schedule: July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985. This is similar to what was observed under the Original Schedule and also is caused by well TT-26 being out of service during these periods.

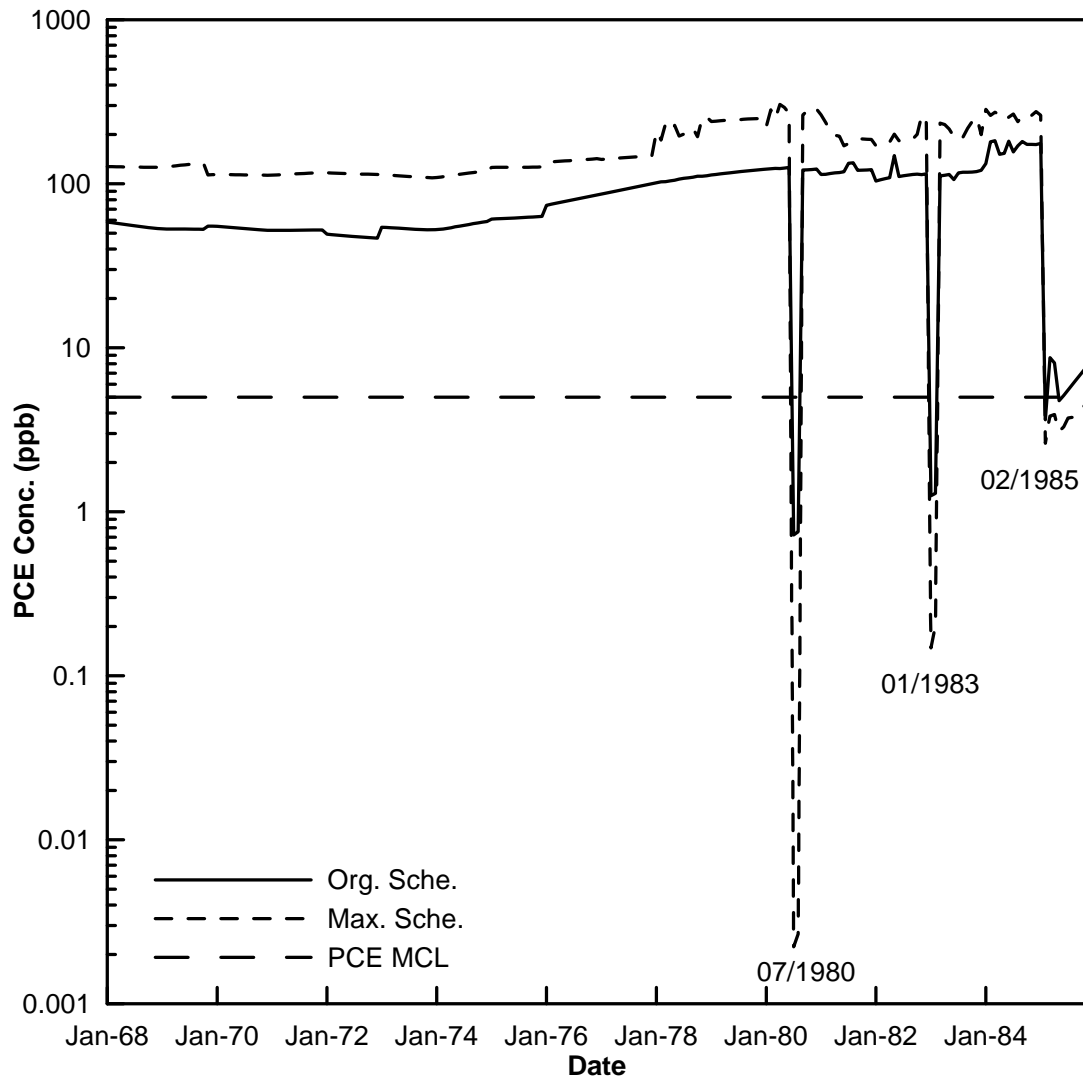


Figure 4.8. PCE concentrations in the WTP under the Original Schedule and the Maximum Schedule for the period of interest

Results given in Figures 4.7 and 4.8 also indicate that after the well TT-26 was shut down in February 1985, the PCE concentration in the WTP was lower than that obtained under the Original Schedule, although the absolute difference is small (less than 4 ppb). This phenomenon is caused by the presence of lower PCE concentrations in the other

water-supply wells. Ten pumping wells were still in service after February 1985 under the Maximum Schedule: well TT-25, TT-23, TT-67A, TT-67B, TT-52A, TT-52B, TT-31A, TT-31B, TT-54A, and TT-54B. Results shown in Figure 4.5 indicate that, besides water-supply wells with PCE concentrations lower than 0.001 ppb and not shown in the figure, the PCE concentrations in all the remaining wells were lower under the Maximum Schedule when compared with the results obtained under the Original Schedule during this period.

The lower PCE concentrations in these pumping wells may be attributed to the following:

- i. According to results given in Figures 4.2, 4.3, and 4.4, the higher pumping rate in well TT-26 under the Maximum Schedule causes the PCE plume to aggregate into a smaller region, which in turn causes lower PCE concentrations in the water-supply wells other than TT-26;
- ii. More contaminant mass is withdrawn and less mass is left in the groundwater system under the Maximum Schedule. According to the ATSDR study, 1.40×10^7 grams of PCE was released into the groundwater system from January 1953 to December 1984. By the time all the pumping operations were terminated (February 1987), 2.45×10^6 grams of PCE was discharged through the water-supply wells under the Original Schedule, while 4.59×10^6 grams of PCE was discharged under the Maximum Schedule as indicated in Table 4.2.

Table 4.2. PCE masses withdrawn under the Original Schedule and the Maximum Schedule

	Total Mass Released (g)	Mass Withdrawn (g)	Percentage (%)
Orig. Sche.	1.40×10^7	2.45×10^6	17.50
Max. Sche.	1.40×10^7	4.59×10^6	32.78

As discussed before, there are 15 months during the period of interest when well TT-26 was out of service and the PCE concentration in the WTP was lower than 5 ppb. In all the other 201 months, PCE concentration in the WTP was higher than the MCL under both the Original Schedule and the Maximum Schedule. A comparison of PCE concentrations in the WTP during those 201 months is summarized in Table 4.3.

Table 4.3. PCE concentrations in the WTP under the Original Schedule and the Maximum Schedule for the period of interest* (Units: ppb)

	Maximum	Minimum	Average
Orig. Sche.	183.04	46.69	86.39
Max. Sche.	304.66	108.76	166.07
Difference	180.75	42.67	79.68

* Data for July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985 are not included.

4.2 Optimization and simulation results for the Minimum Schedule I

Similar to the Maximum Schedule, PSOpS was run to obtain the Minimum Schedule I to obtain the “latest” PCE MCL arrival time in the Tarawa Terrace WTP. The results obtained under the Minimum Schedule I indicate that well TT-26 pumped at a lowest possible rate for most of the time period (Figure 4.9), which implies that well TT-26 was not put into operation unless no other water-supply well was available to provide the required total demand. The reason for this is clear since the PCE concentration in well TT-26 is significantly higher than those in other pumping wells. For most of the simulation period, the lower PCE concentration in the WTP can be realized by reducing the pumping rate of well TT-26. However, there are exceptions to this during the period of late 1970s and early 1980s, which will be discussed in the following section.

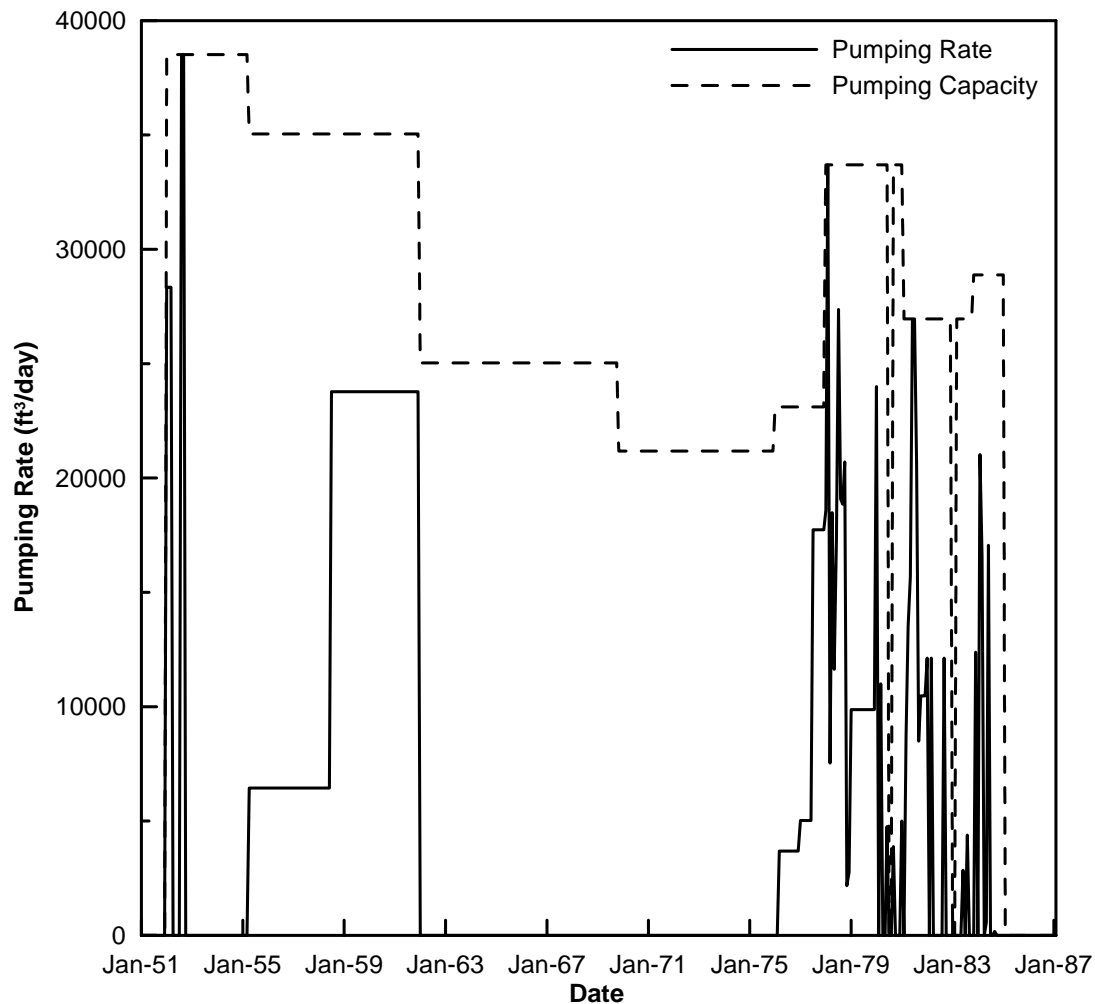


Figure 4.9. Pumping rate and pumping capacity of well TT-26 under the Minimum Schedule I

4.2.1 PCE distribution in the groundwater system

Similar to the Maximum Schedule results presented in Figures 4.2, 4.3, and 4.4, the PCE distributions in the subsurface system around the Tarawa Terrace area and the vicinity under the Original Schedule and the Minimum Schedule I are compared in Figures 4.10, 4.11 and 4.12. The notation used in these figures is the same as used for Figures 4.2 – 4.4.

Results presented in Figures 4.10, 4.11, and 4.12 indicate that the Minimum Schedule I also causes a change of PCE distribution in the groundwater system. Opposite to what has been observed under the Maximum Schedule, the contaminant plume under the Minimum Schedule I is dispersed to a larger area, and the front of the plume is more away from the location of well TT-26. Therefore, PCE concentrations in some wells other than well TT-26 are expected to be higher, and the PCE concentration in TT-26 is expected to be lower.

According to the results presented in these figures, the PCE concentration near well TT-26 is still relatively high due to its closeness to the contaminant source, which causes a higher PCE concentration in well TT-26 when compared to the other wells. Therefore, as discussed in previous section, well TT-26 was pumped at the lowest possible rates for most of the time under the Minimum Schedule I to lower the PCE concentration in the WTP.

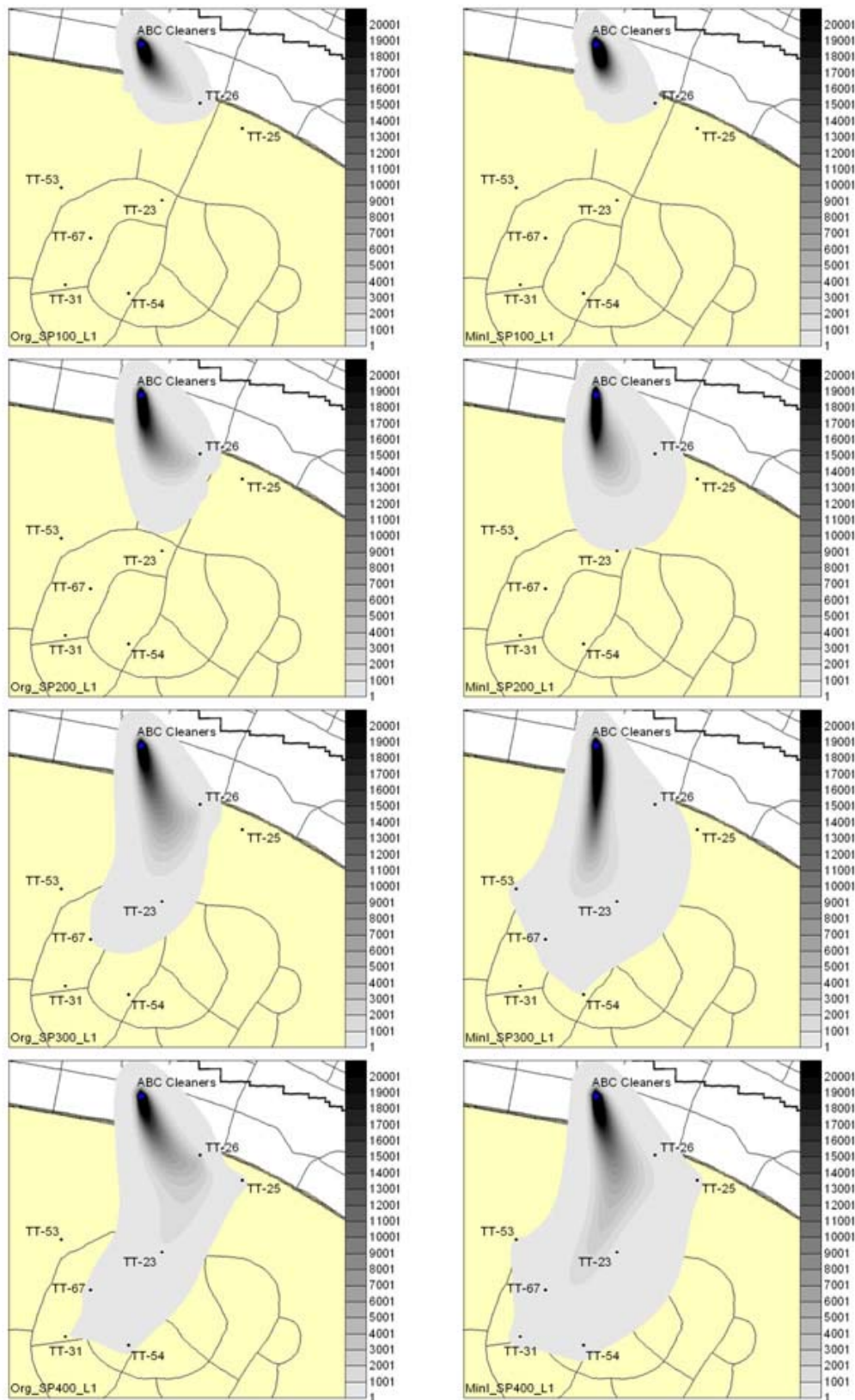


Figure 4.10. Comparison of PCE distribution in Layer 1 under the Original Schedule and the Minimum Schedule I (Units: ppb)

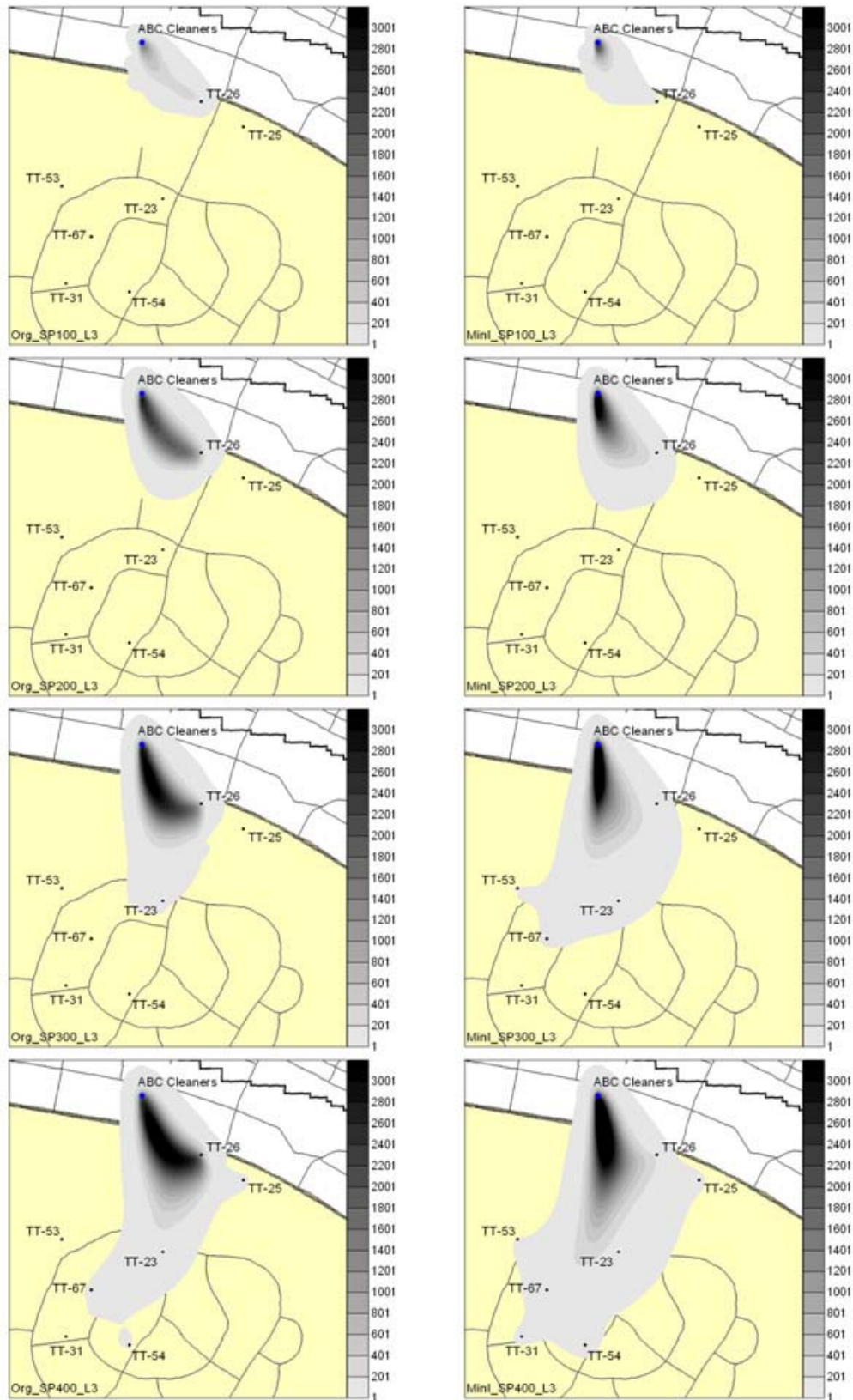


Figure 4.11. Comparison of PCE distribution in Layer 3 under the Original Schedule and the Minimum Schedule I (Units: ppb)

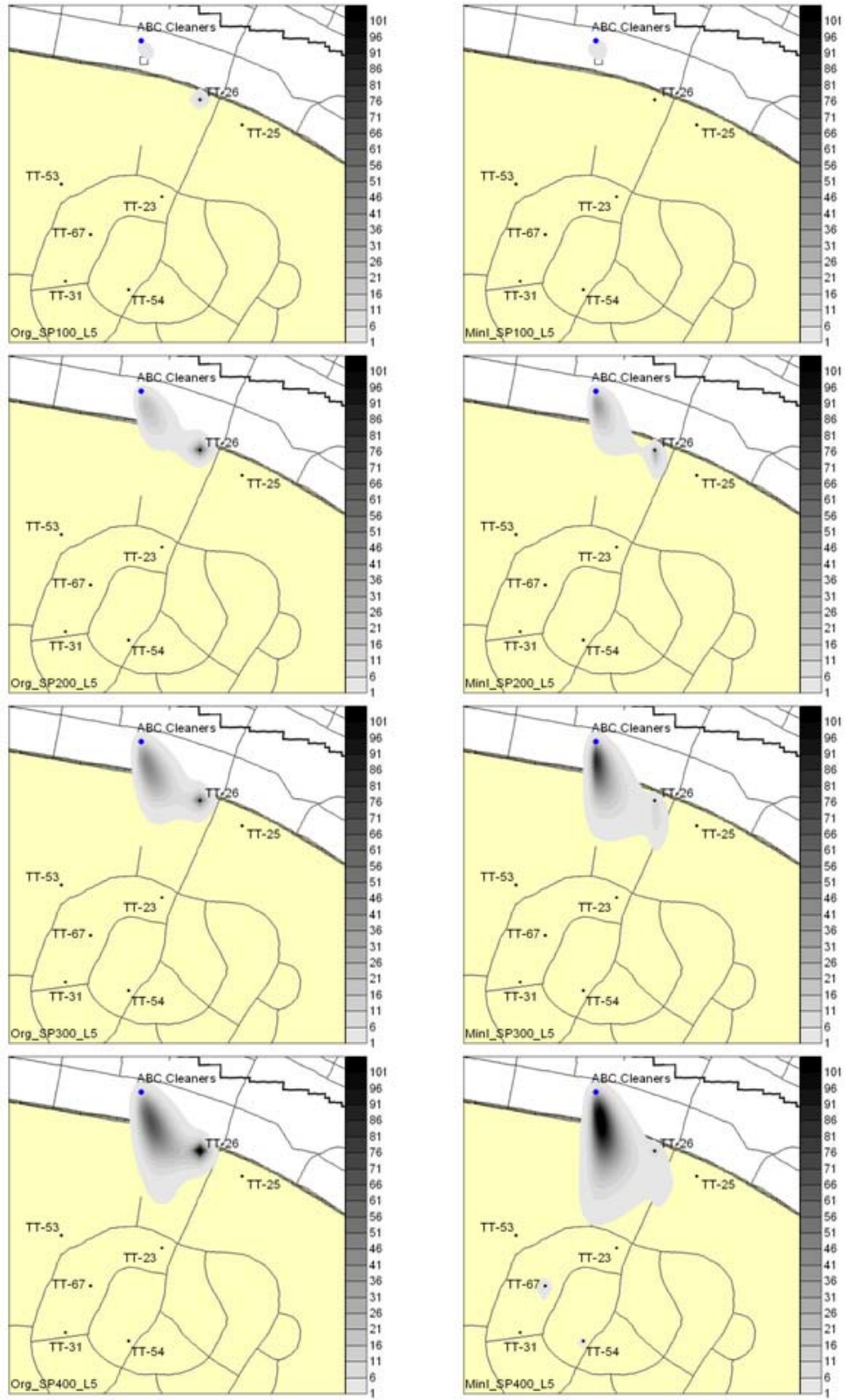


Figure 4.12. Comparison of PCE distribution in Layer 5 under the Original Schedule and the Minimum Schedule I (Units: ppb)

4.2.2 PCE concentration in the water-supply wells

The output of the MT3DMS simulation under the Minimum Schedule I provide PCE concentrations in the water-supply wells. These results show higher PCE concentrations in some of the pumping wells other than TT-26. Due to the large number of pumping wells with PCE concentrations higher than 0.001 ppb, only wells with PCE concentrations higher than 5 ppb are shown in Figure 4.13. Another version of this figure emphasizing the period of interest is shown in Figure 4.14.

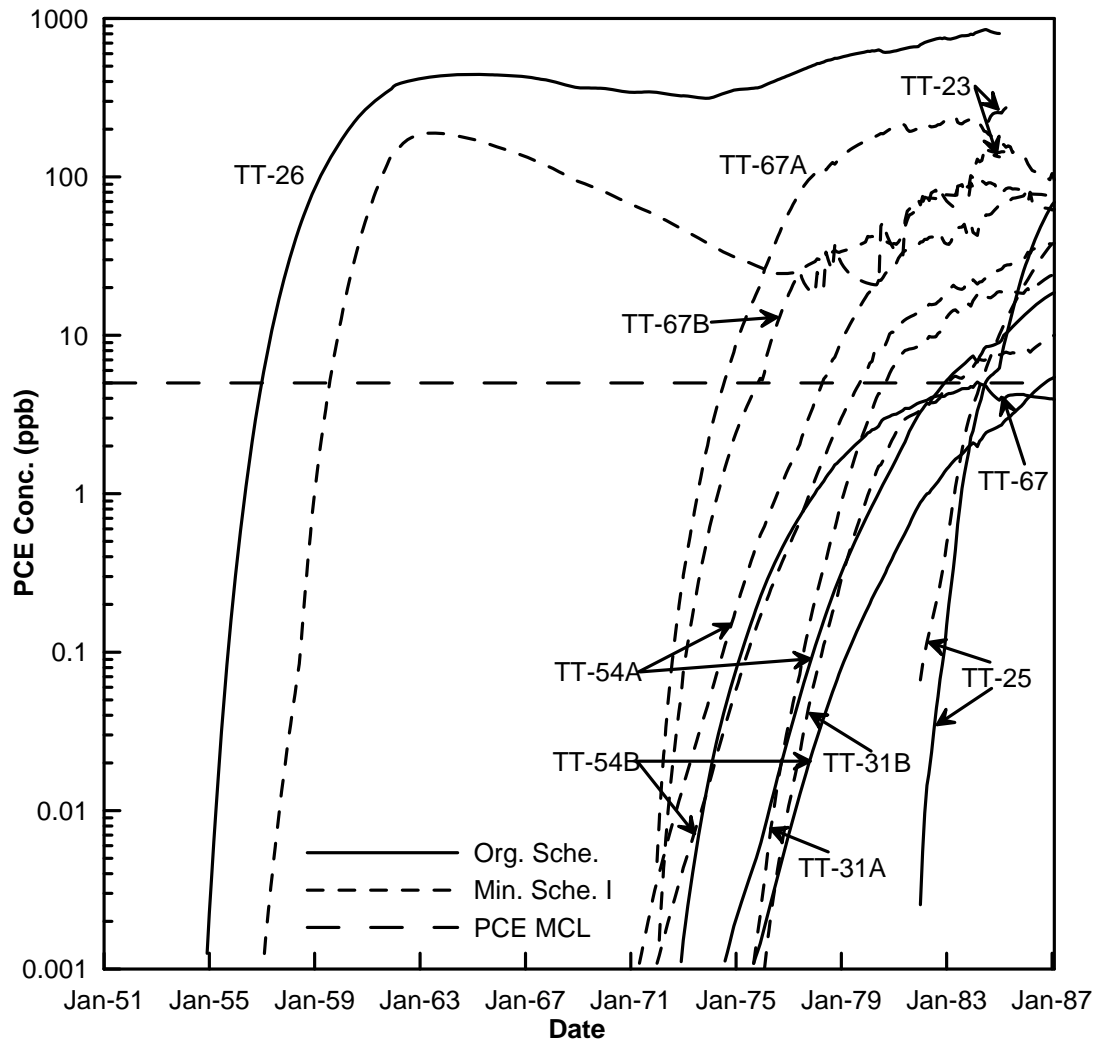


Figure 4.13. PCE concentrations in water-supply wells under the Original Schedule and the Minimum Schedule I

From the results given in Figures 4.13 and 4.14, one may observe the following:

- i. Instead of six water-supply wells (TT-26, TT-23, TT-25, TT-67, TT-54A, and TT-54B) having PCE concentrations higher than 5 ppb as seen with the Maximum Schedule, nine pumping wells have PCE concentrations more than 5 ppb under the Minimum Schedule I. These wells are TT-26, TT-23, TT-25,

TT-31A, TT-31B, TT-54A, TT-54B, TT-67A, and TT-67B. As discussed in the previous section, this is caused by the generation of a more dispersed contaminant plume under the Minimum Schedule I;

- ii. PCE concentration in well TT-26 is always lower under the Minimum Schedule I when compared to that obtained under the Original Schedule throughout the simulation period;
- iii. Well TT-26 is the first well to have a PCE concentration over PCE MCL. During the first half of the simulation period, well TT-26 is the only well with a PCE concentration higher than 5 ppb. Therefore, well TT-26 is still critical to the PCE MCL arrival time in the WTP;
- iv. PCE concentration in well TT-26 exceeded 5 ppb in August 1959 under the Minimum Schedule I, which is 31 months later than the case for the Original Schedule (January 1957). This delay would cause a “late” PCE MCL arrival time in the WTP as well;
- v. The PCE concentration in well TT-26 is no longer dominant during the second half of the simulation period under the Minimum Schedule I. PCE concentrations in well TT-23, TT-67A, and TT-67B are sometimes higher than that in well TT-26. Higher PCE concentrations in these pumping wells also explain why well TT-26 is not always pumping at the lowest possible rates towards the end of the simulation period – with several pumping wells having high PCE concentration in them, the Minimum Schedule I is managed in a way that the plume front is not led to any particular water-supply well.

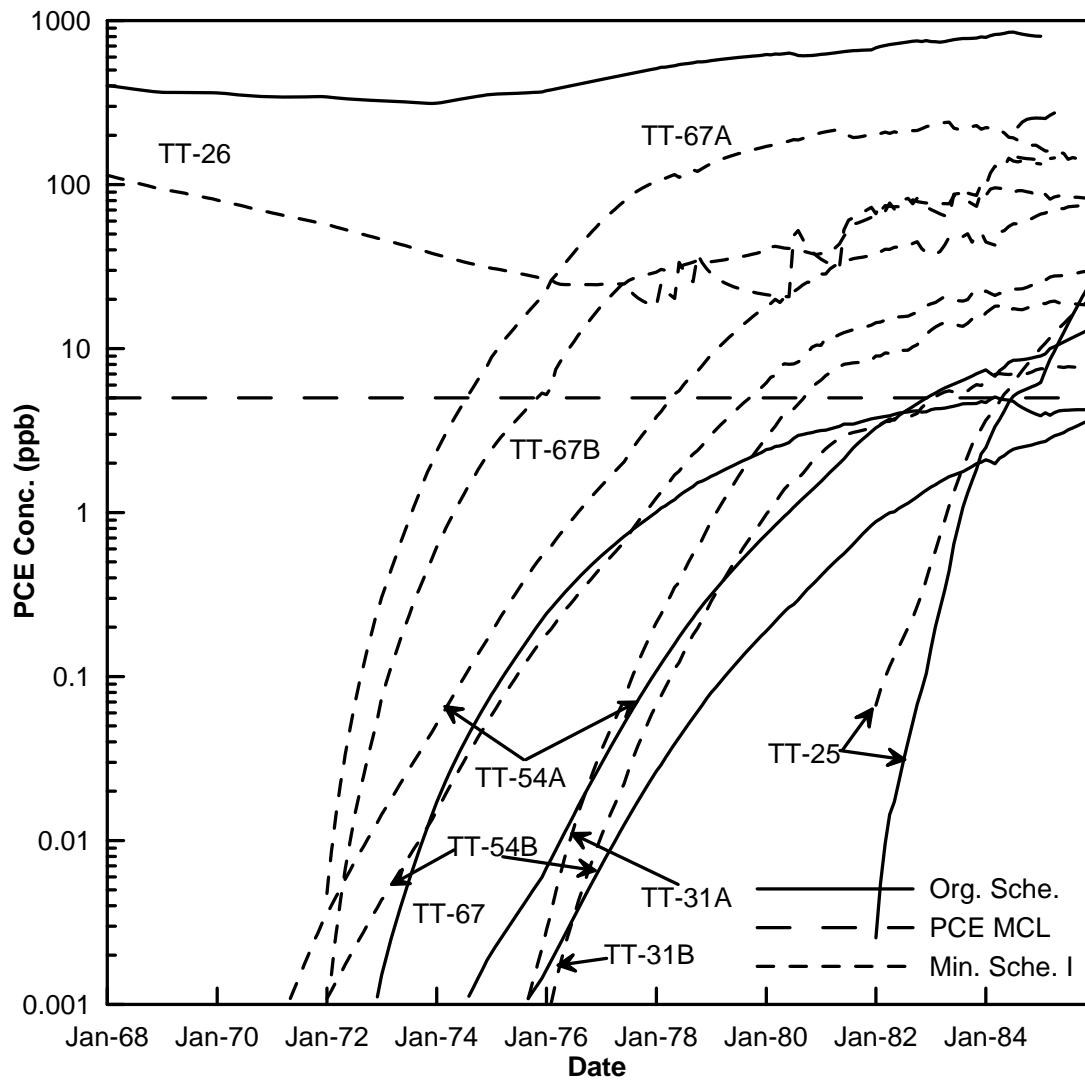


Figure 4.14. PCE concentrations in water-supply wells under the Original Schedule and the Minimum Schedule I for the period of interest

4.2.3 PCE concentration in the WTP

The PCE concentration in the Tarawa Terrace WTP under the Minimum Schedule I is calculated using Equation (2.3) and is shown in Figures 4.15 and 4.16.

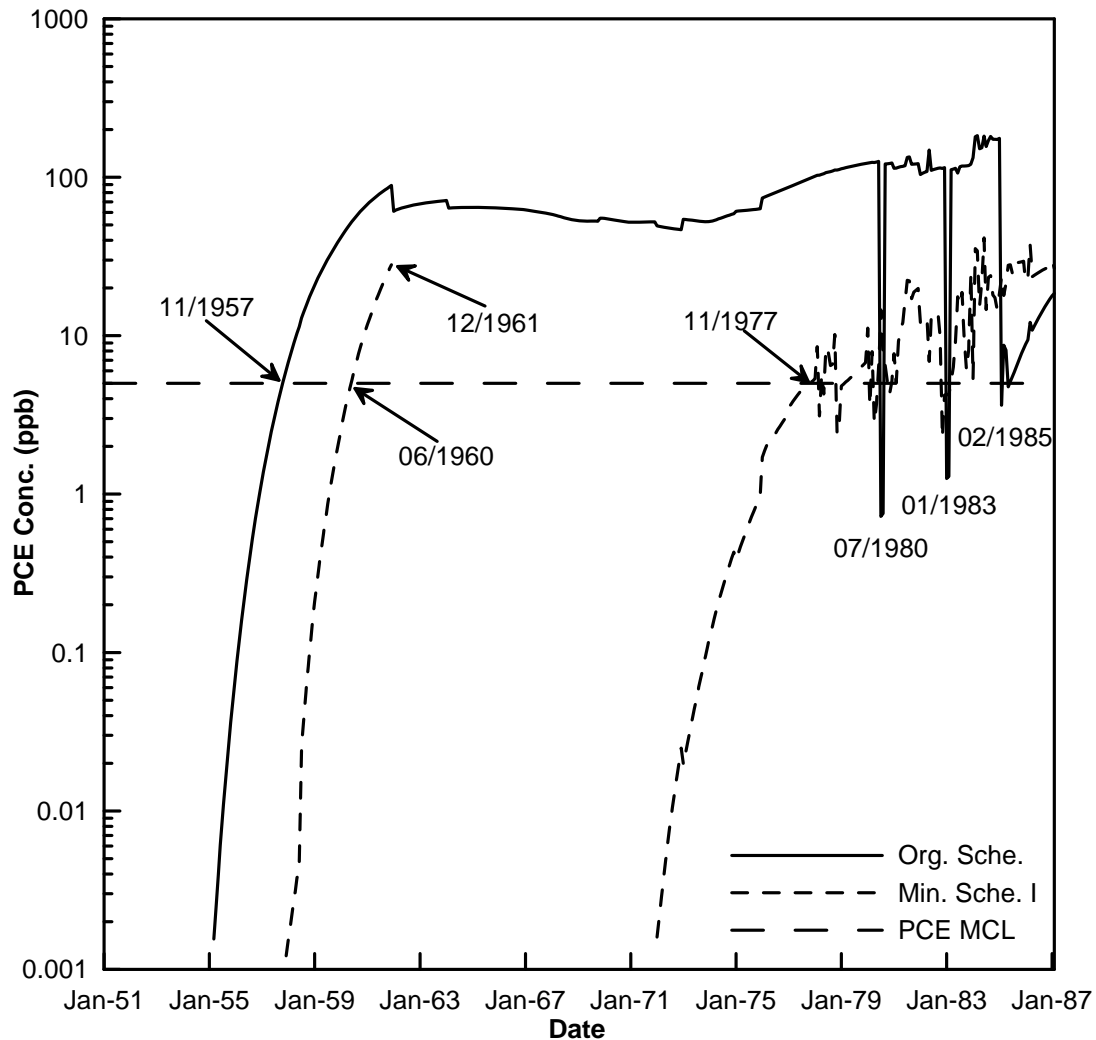


Figure 4.15. PCE concentrations in the WTP under the Original Schedule and the Minimum Schedule I

The results presented in Figures 4.15 and 4.16 lead to the following observations:

- i. The PCE concentration in the WTP under the Minimum Schedule I is lower than that obtained under the Original Schedule except for the period after February 1985;
- ii. The PCE concentration in the WTP reached 5 ppb in June 1960 under the Minimum Schedule I, which is 31 months later than the arrival time of the Original Schedule. This is due to the lower PCE concentration and lower pumping rate in well TT-26 under the Minimum Schedule I. According to Figure 4.13, by the time the PCE concentration in the WTP reached 5 ppb, the PCE concentrations in the supply wells other than TT-26 were still negligible. Therefore, well TT-26 is the critical well affecting the PCE MCL arrival time in the WTP;
- iii. Under the Minimum Schedule I, the PCE concentration in the WTP increased

steadily until December 1961, when the PCE concentration dropped below trace levels due to zero-pumping in well TT-26. The concentration reached 5 ppb again in November 1977. Between January 1962 and December 1971, the PCE concentration in the WTP was lower than 0.001 ppb and therefore is not shown in these figures;

- iv. The sudden PCE concentration drops that were observed during periods of July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985 under the Original Schedule were not obvious under the Minimum Schedule I for two reasons. First the overall PCE concentration level in the WTP is very low under the Minimum Schedule I. Second, the PCE concentration in well TT-26 is no longer dominant as shown in Figure 4.14.

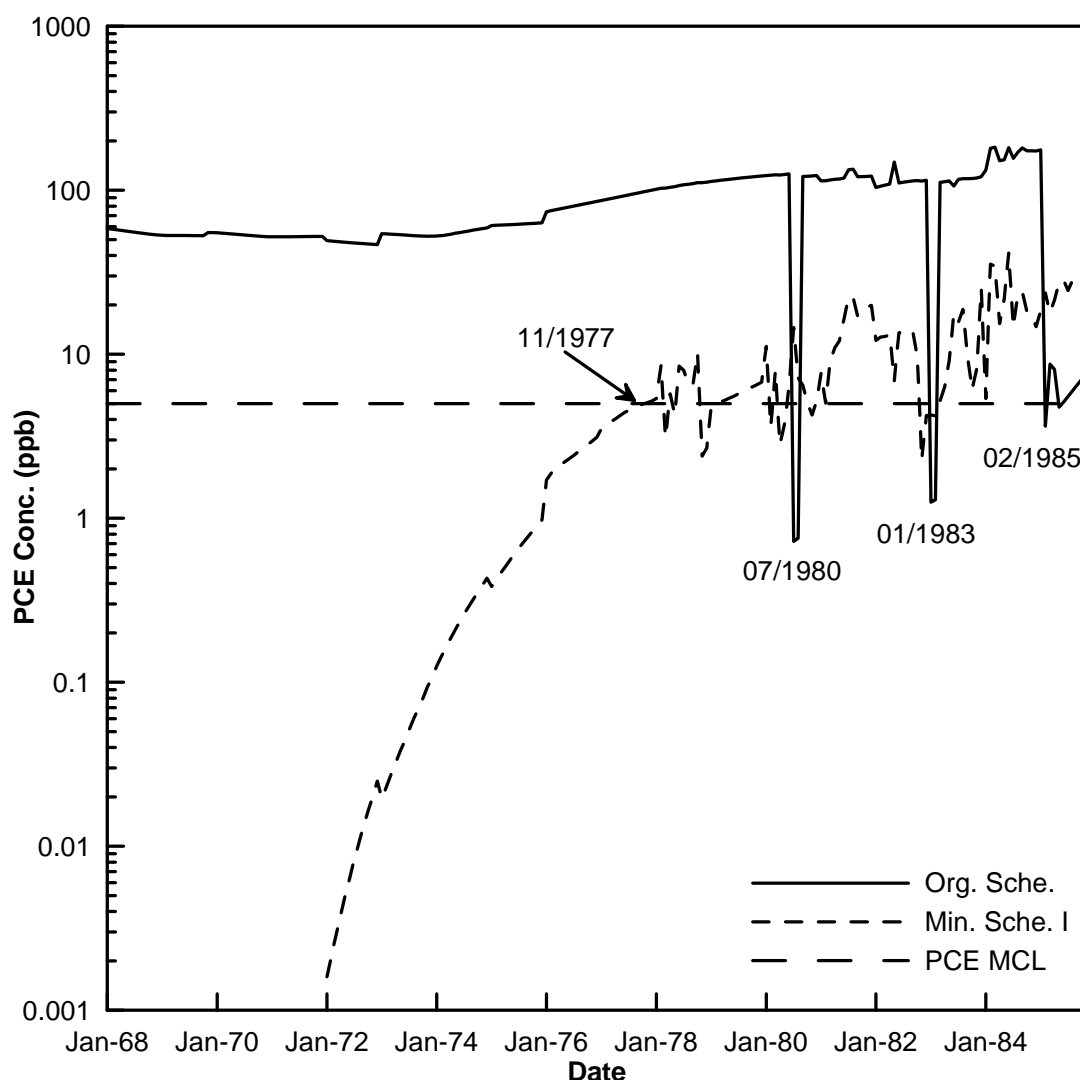


Figure 4.16. PCE concentrations in the WTP under the Original Schedule and the Minimum Schedule I for the period of interest

Another observation that can be made from the results presented in Figures 4.15 and 4.16

is that during the last 11 months of the period of interest the PCE concentrations in the WTP under the Minimum Schedule I are slightly higher than those obtained under the Original Schedule, which is in contrast to the results obtained under the Maximum Schedule. The reason for this is the higher PCE concentrations in some water-supply wells other than well TT-26 (i.e., well TT-67A and TT-67B). The higher PCE concentrations in these pumping wells may be caused by the following factors:

- i. As shown in Table 4.4, by the end of the period of interest, less contaminant mass was extracted from the groundwater system under the Minimum Schedule I, and more mass was left in the aquifer, which causes higher PCE concentrations in the water-supply wells;
- ii. The Minimum Schedule I causes a more dispersed contaminant plume in the groundwater system. While PCE concentration in well TT-26 is decreased, the PCE concentrations in some other wells are increased.

Table 4.4. PCE masses withdrawn under the Original Schedule and the Minimum Schedule I

	Total Mass Released (g)	Mass Withdrawn (g)	Percentage (%)
Orig. Sche.	1.40×10^7	2.45×10^6	17.50
Min. Sche. I	1.40×10^7	1.98×10^5	1.41

The Minimum Schedule I yields lower PCE concentrations in the WTP during the period of interest (Table 4.5). To keep this comparison consistent with the previous comparison made for the Maximum Schedule, the concentration distribution obtained from the 15 months when well TT-26 was out of service was not included in this analysis. The results shown in Table 4.5 indicate that the average PCE concentration in the WTP under the Minimum Schedule I is 5.01 ppb, which is quite close to the 5 ppb MCL of PCE.

Table 4.5. PCE concentrations in the WTP under the Original Schedule and the Minimum Schedule I for the period of interest* (Units: ppb)

	Maximum	Minimum	Average
Orig. Sche.	183.04	46.69	86.39
Min. Sche. I	41.36	7.84×10^{-8}	5.01
Difference	158.48	46.69	81.39

* Data for July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985 are not included.

4.3 Optimization and simulation results for the Minimum Schedule II

The “late” PCE MCL arrival time in the WTP can be obtained through MODFLOW and MT3DMS simulations using the Minimum Schedule I developed earlier. These results indicate that under Minimum Schedule I, well TT-26 was out of service for a long period of time, which is unrealistic based on the historical records and also considering that well

TT-26 was one of the major water-supply wells in the Tarawa Terrace area. Therefore, a third PSOpS simulation was conducted to obtain a pumping schedule which may still yield the “latest” arrival time but at the same time be closer to the historical data on the schedule of operations at the site. To achieve this, one more constraint was added to the optimization model. The pumping rate in well TT-26 is restricted not to be less than 25% of its pumping capacity at any time when the pumping well was in service. The pumping rate of well TT-26 obtained for this case is shown in Figure 4.17. Similar to the Minimum Schedule I, the Minimum Schedule II pumping rate for well TT-26 also is the lowest possible during the first half of the simulation period.

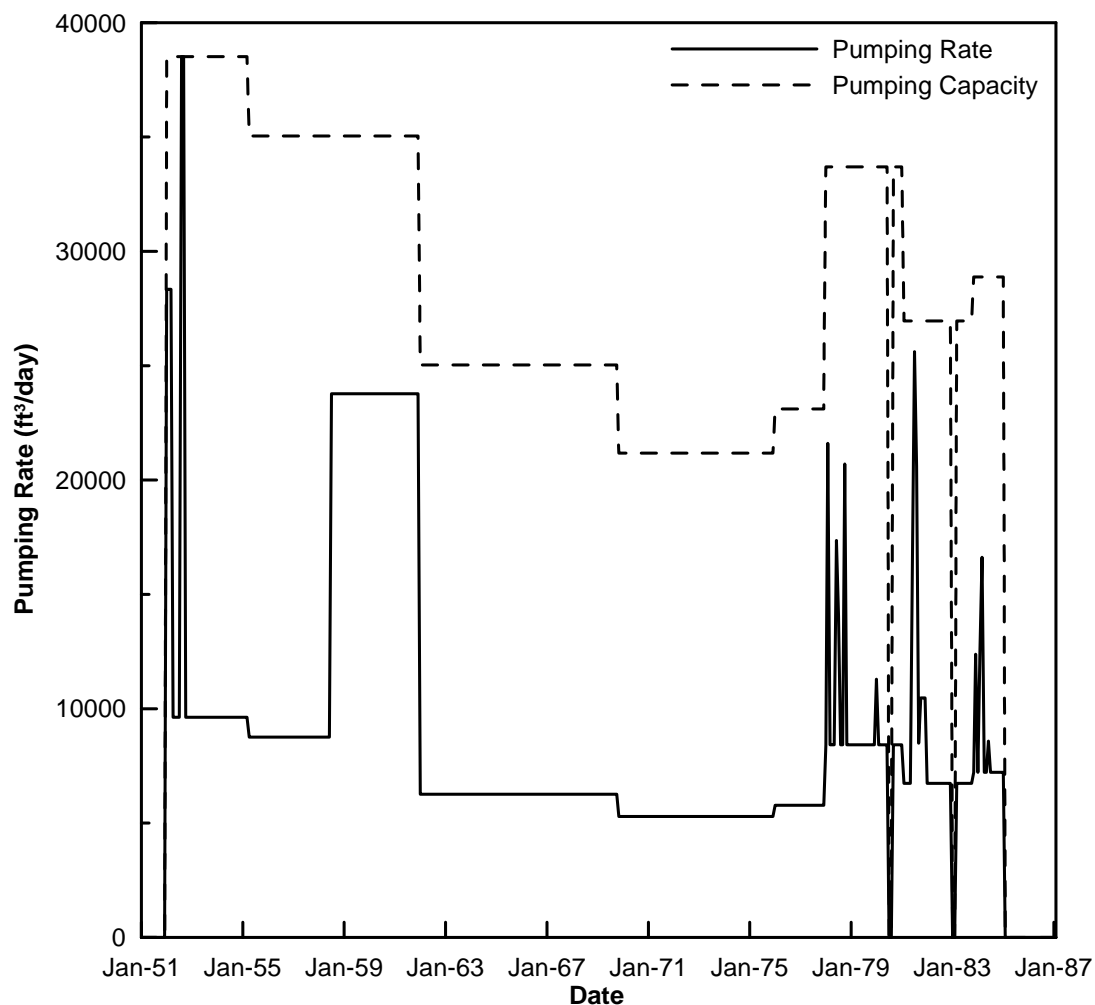


Figure 4.17. Pumping rate and pumping capacity of well TT-26 under the Minimum Schedule II

4.3.1 PCE distribution in the groundwater system

The PCE distribution in the subsurface system in the Tarawa Terrace area and vicinity under the Original Schedule and the Minimum Schedule II are compared in Figures 4.18, 4.19, and 4.20 for different stress periods. A comparisons of PCE distributions obtained under the Minimum Schedules I and II are shown in Figures 4.21, 4.22, and 4.23. The

notations used in these figures are the same as used in Figure 4.2.

A comparison of Figures 4.10, 4.11, and 4.12 and Figures 4.18 through 4.23 indicate that the Minimum Schedule II also causes the PCE plume to be more dispersed than the Original Schedule, but not as much as the Minimum Schedule I. This is because the average pumping rate in well TT-26 under the Minimum Schedule II is lower than that obtained under the Original Schedule, but higher than the average pumping rate obtained under the Minimum Schedule I. Therefore, one may expect the PCE concentrations in well TT-26 and the WTP under the Minimum Schedule II to be between those obtained under the Original Schedule and the Minimum Schedule I.

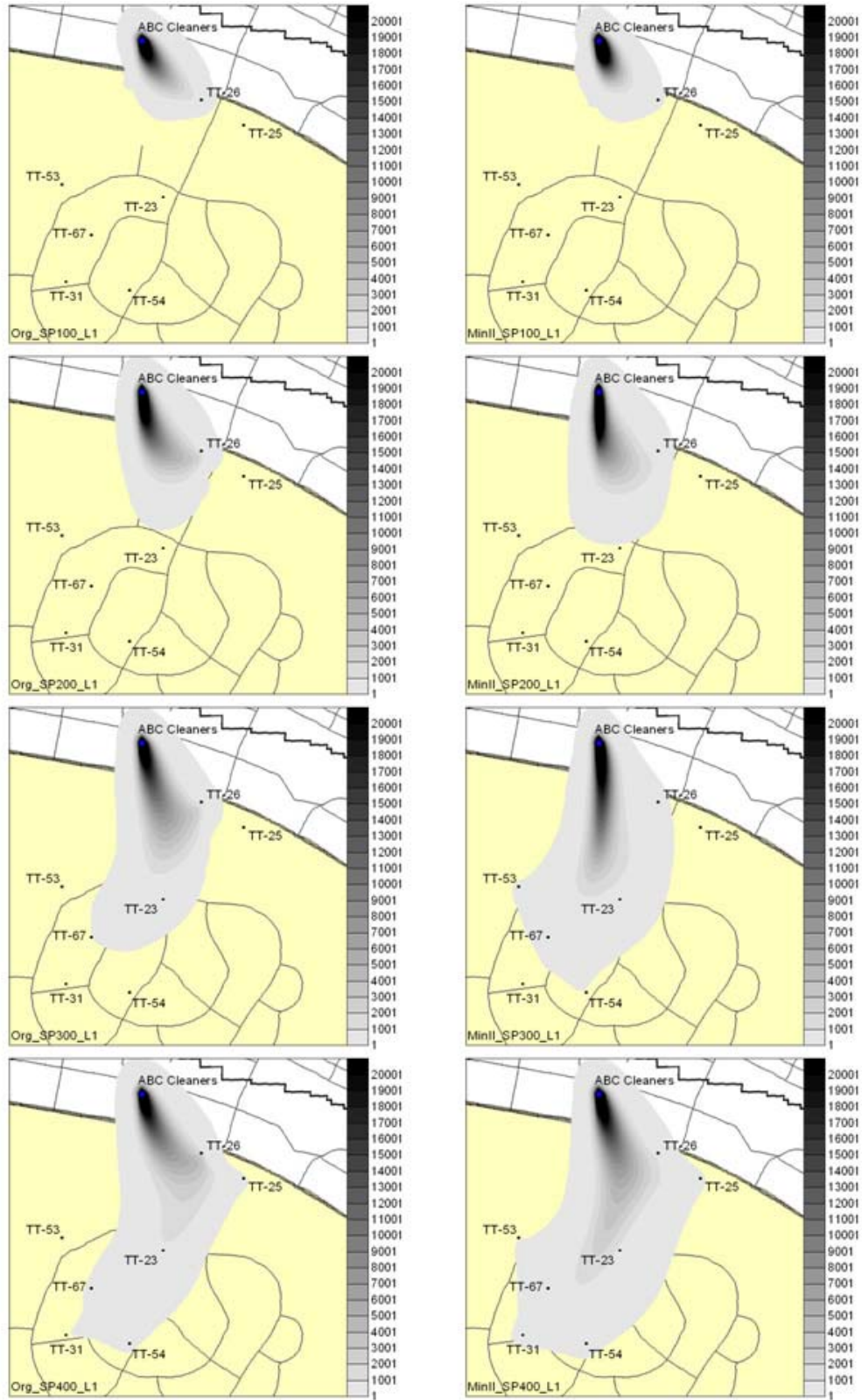


Figure 4.18. Comparison of PCE distribution in Layer 1 under the Original Schedule and the Minimum Schedule II (Units: ppb)

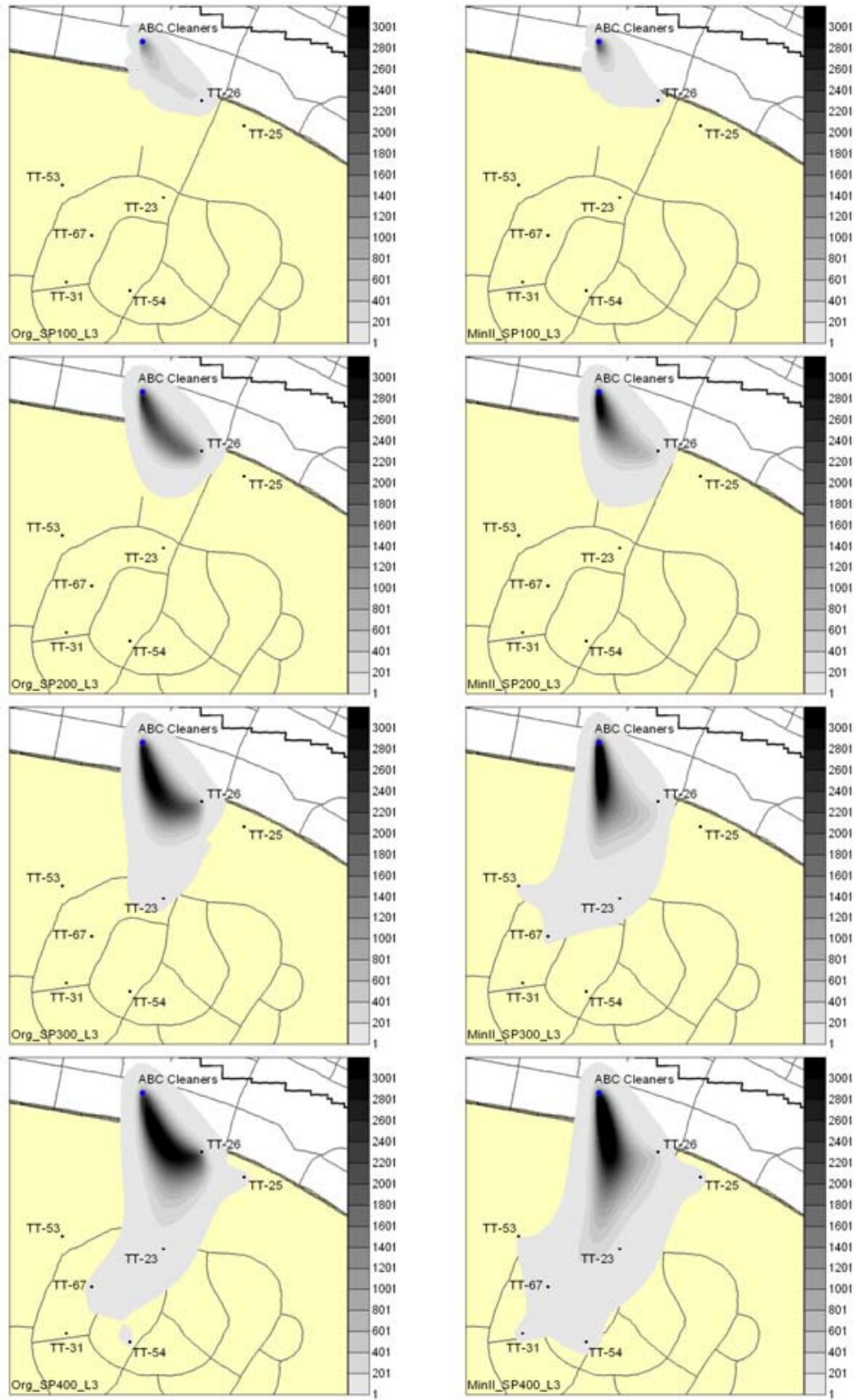


Figure 4.19. Comparison of PCE distribution in Layer 3 under the Original Schedule and the Minimum Schedule II (Units: ppb)

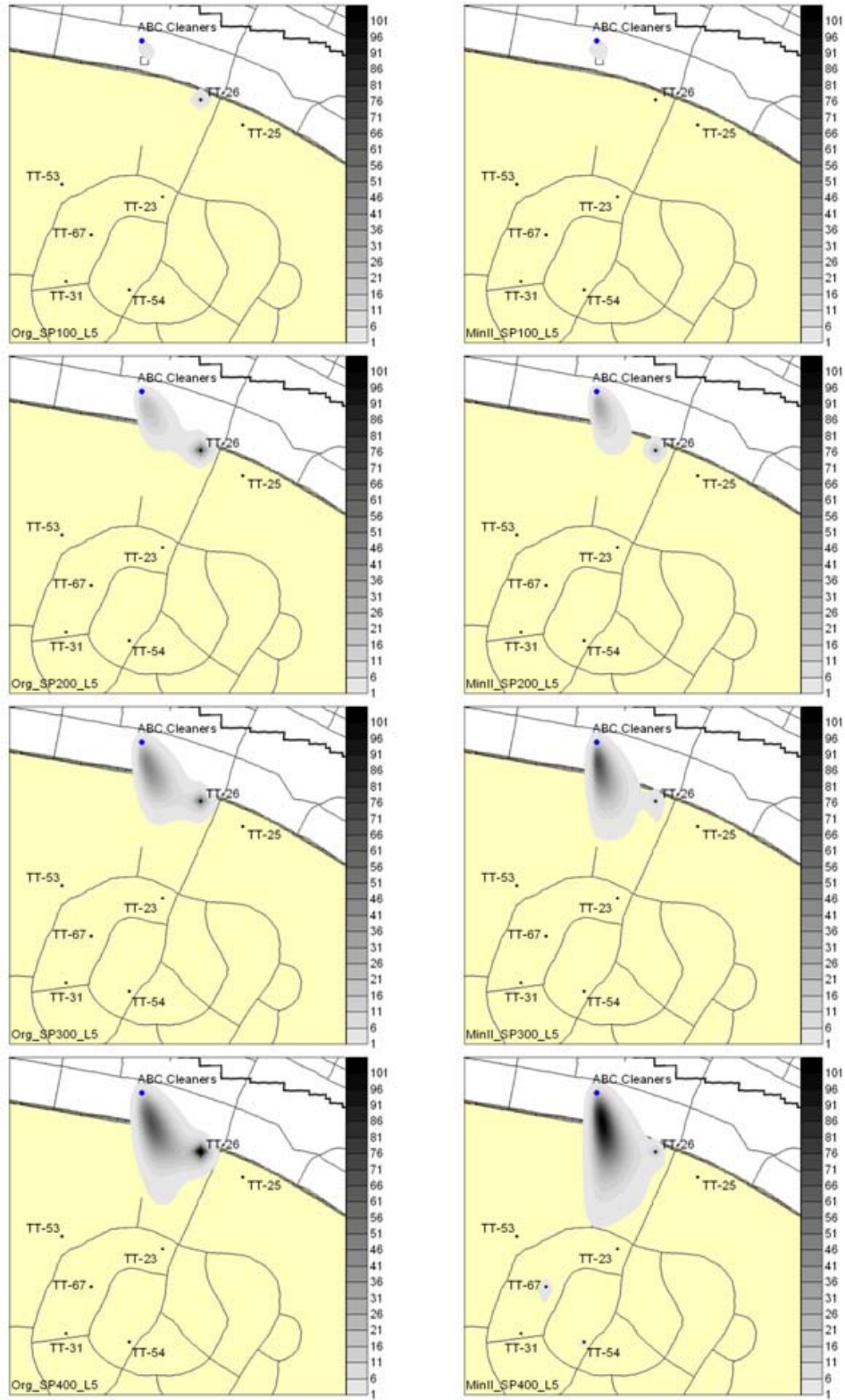


Figure 4.20. Comparison of PCE distribution in Layer 5 under the Original Schedule and the Minimum Schedule II (Units: ppb)

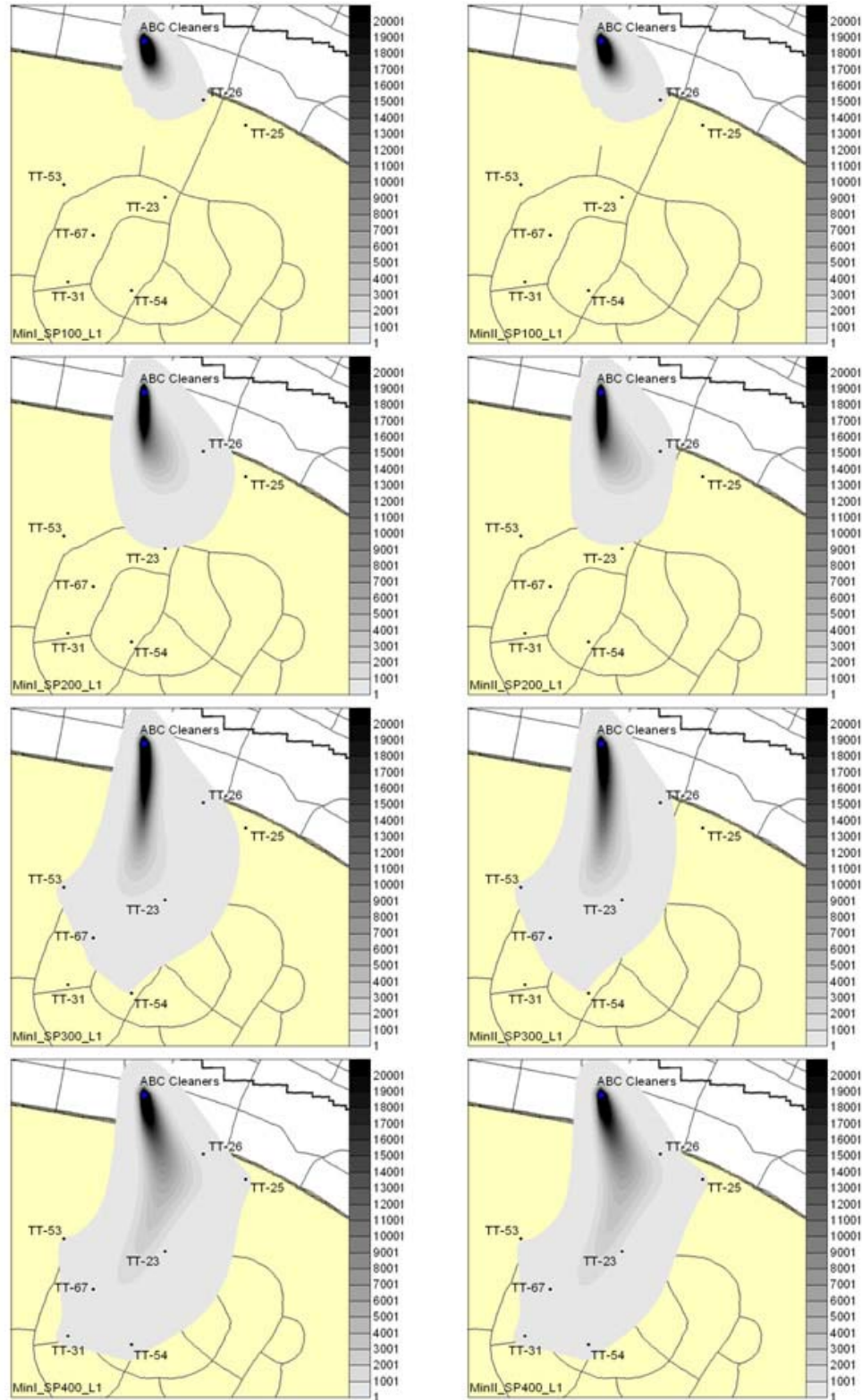


Figure 4.21. Comparison of PCE distribution in Layer 1 under the Minimum Schedule I and the Minimum Schedule II (Units: ppb)

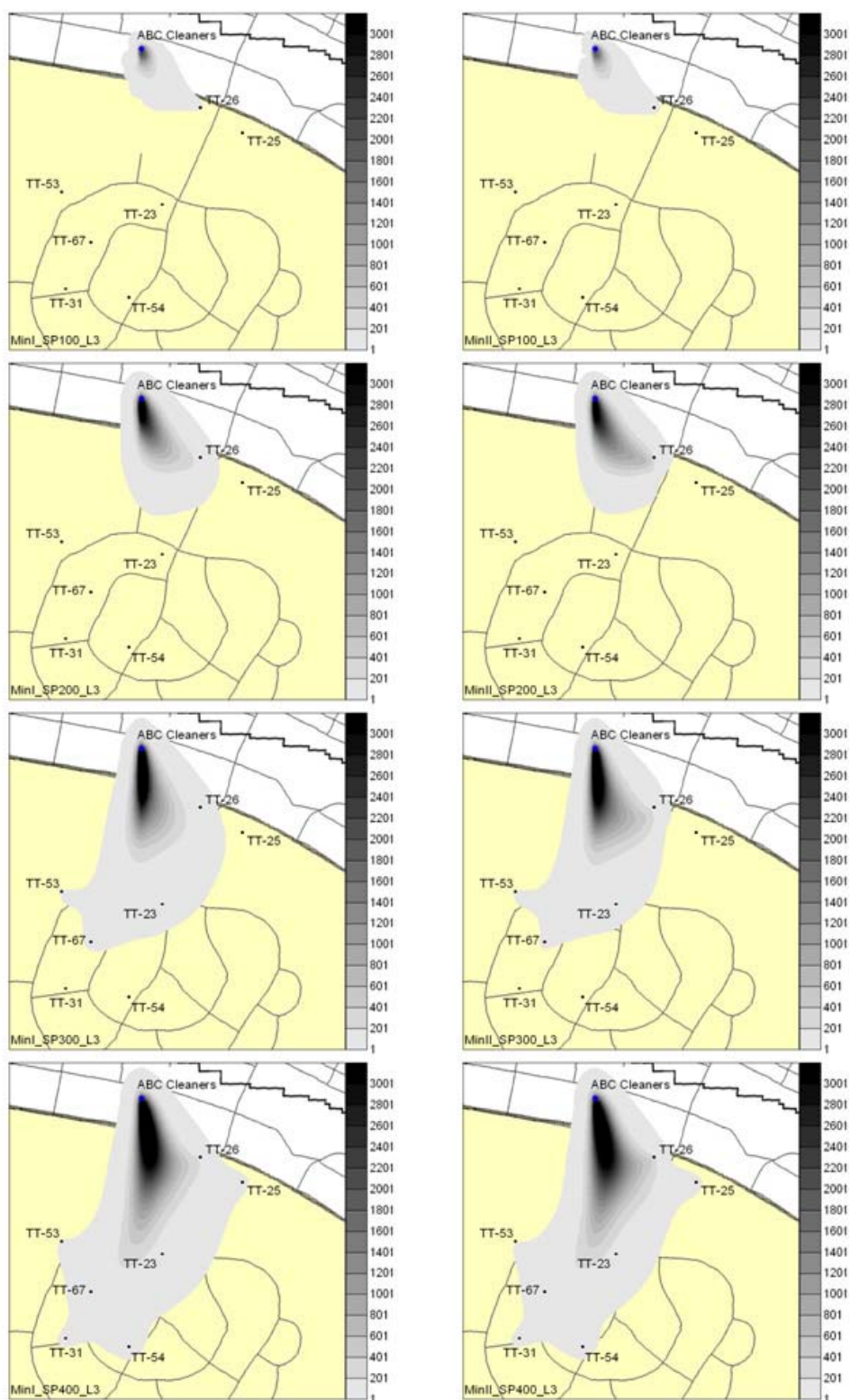


Figure 4.22. Comparison of PCE distribution in Layer 3 under the Minimum Schedule I and the Minimum Schedule II (Units: ppb)

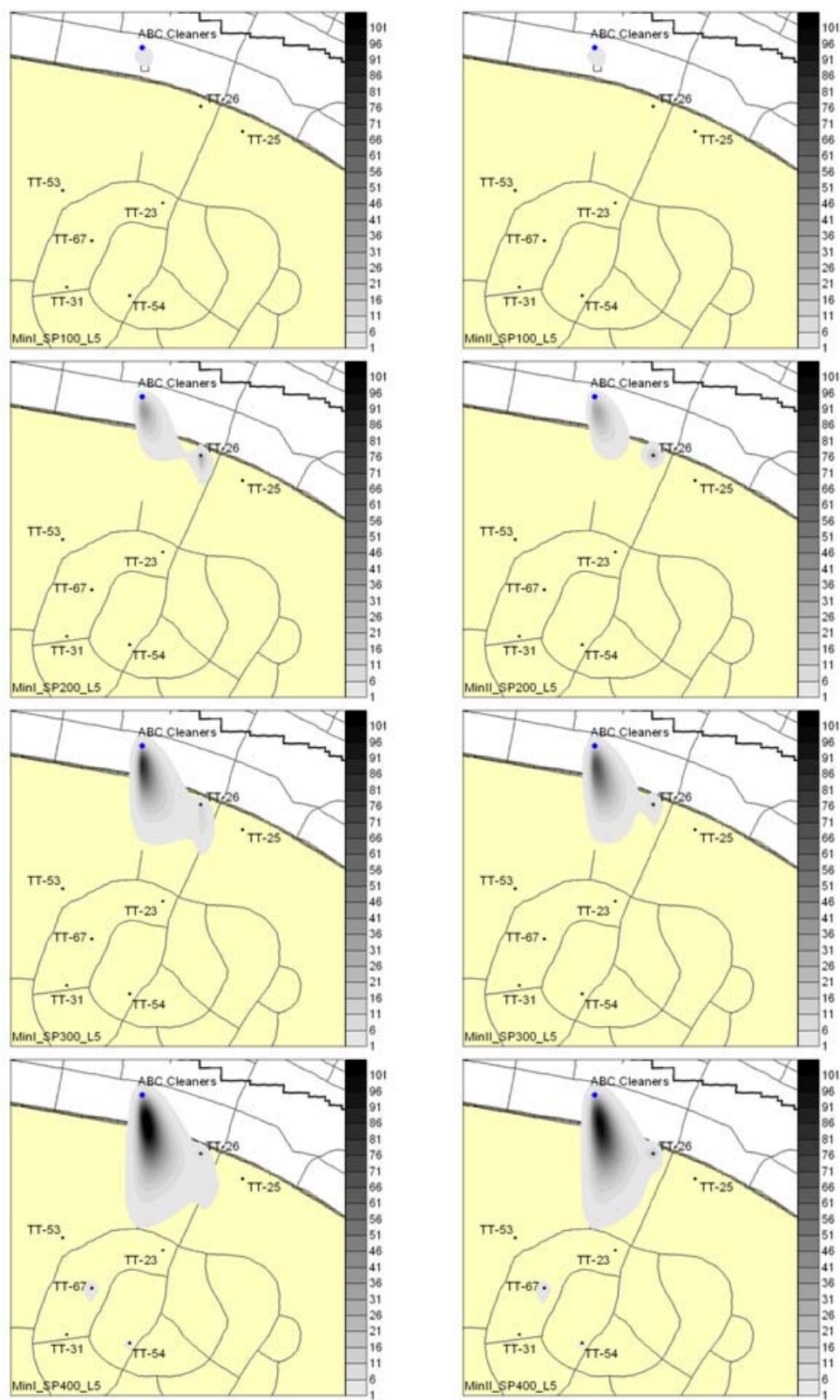


Figure 4.23. Comparison of PCE distribution in Layer 5 under the Minimum Schedule I and the Minimum Schedule II (Units: ppb)

4.3.2 PCE concentration in the water-supply wells

Similar to the results presented in Figures 4.13 and 4.14, PCE concentrations in the water-supply wells which had PCE concentrations of more than 5 ppb are plotted in Figures 4.24 and 4.25 for the Minimum Schedule II. A comparison of the PCE concentrations in the major water-supply wells is shown in Figure 4.26.

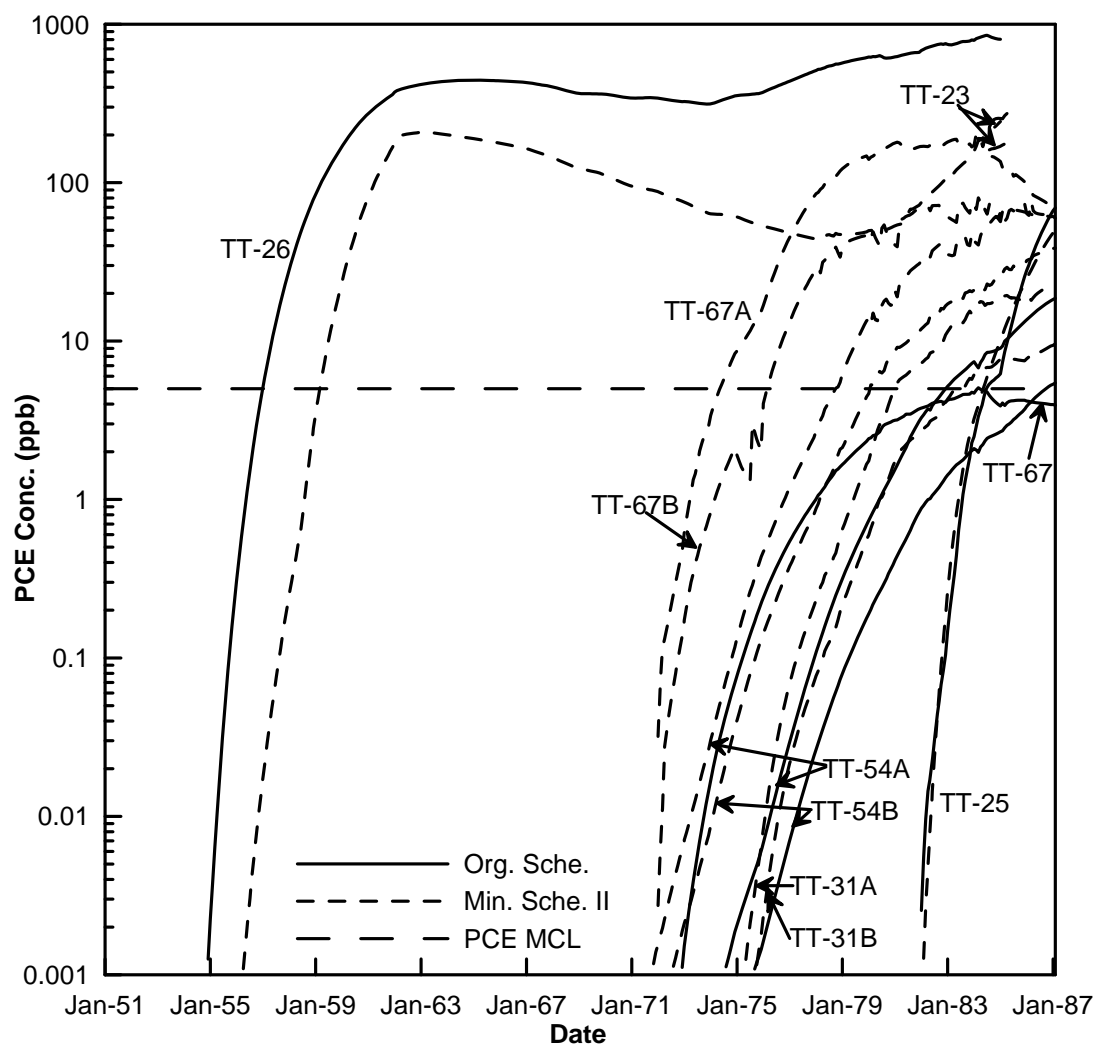


Figure 4.24. PCE concentrations in water-supply wells under the Original Schedule and the Minimum Schedule II

The results summarized in Figures 4.24, 4.25, and 4.26 show that the PCE concentration distribution in the pumping wells under the Minimum Schedule II is similar to the distribution obtained under the Minimum Schedule I. The only difference for this case is that, the PCE concentration in well TT-26 under the Minimum Schedule II is always higher than that obtained under the Minimum Schedule I for most of the period of interest, while the PCE concentrations in some other pumping wells are slightly higher than those obtained under the Minimum Schedule I (Figure 4.26). This is because, as discussed in the previous section, the continuous operation of well TT-26 yields a less

dispersed PCE plume in the groundwater system and the contaminant plume is more directed towards the well TT-26.

The higher PCE concentrations in well TT-26 cause a relatively early PCE MCL arrival time at this location. According to the simulation results, the PCE concentration in well TT-26 reached MCL in March 1959 under the Minimum Schedule II, which is five months earlier than that obtained under the Minimum Schedule I (August 1959). Thus, an earlier PCE MCL arrival time in the WTP is expected for the Minimum Schedule II.

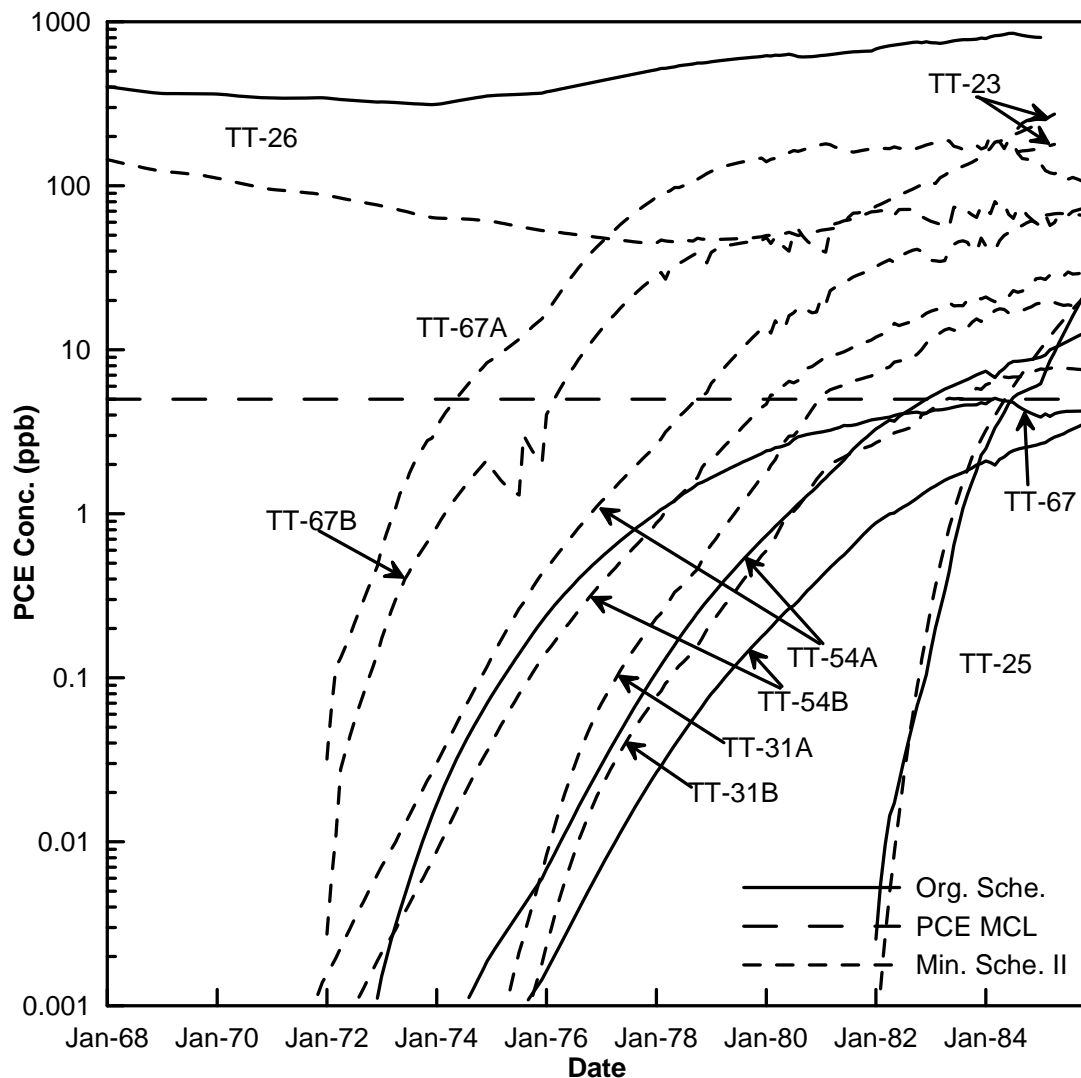


Figure 4.25. PCE concentrations in the major water-supply wells under the Original Schedule and the Minimum Schedule II for the period of interest

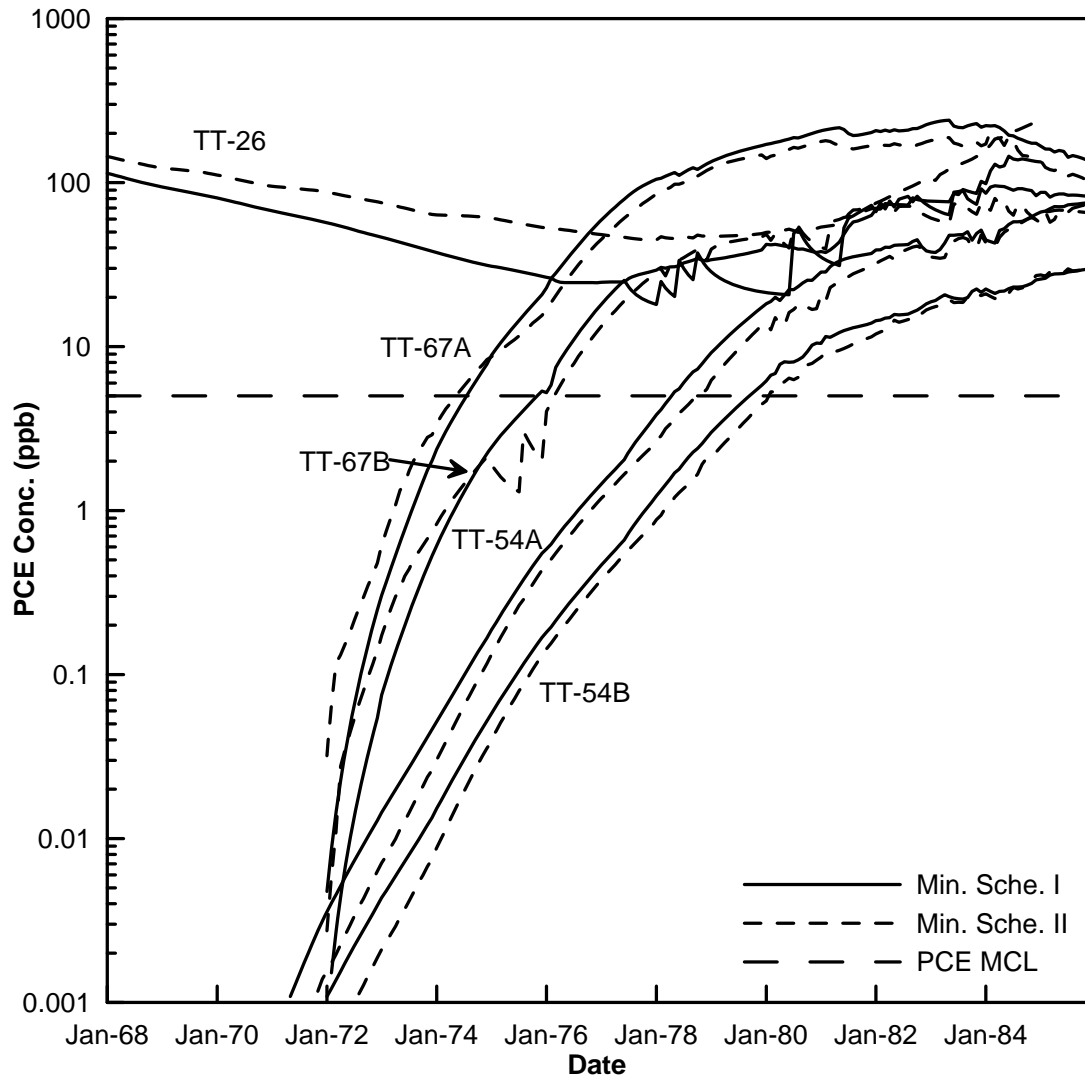


Figure 4.26. PCE concentrations in the major water-supply wells under the Minimum Schedule I and the Minimum Schedule II for the period of interest

4.3.3 PCE concentration in the WTP

PCE concentration in the Tarawa Terrace WTP under the Minimum Schedule II is calculated and presented in Figures 4.27 and 4.28. To illustrate the difference of the PCE concentration between the two minimum schedules, PCE concentration obtained in the WTP under the Minimum Schedule I is shown in these figures as well.

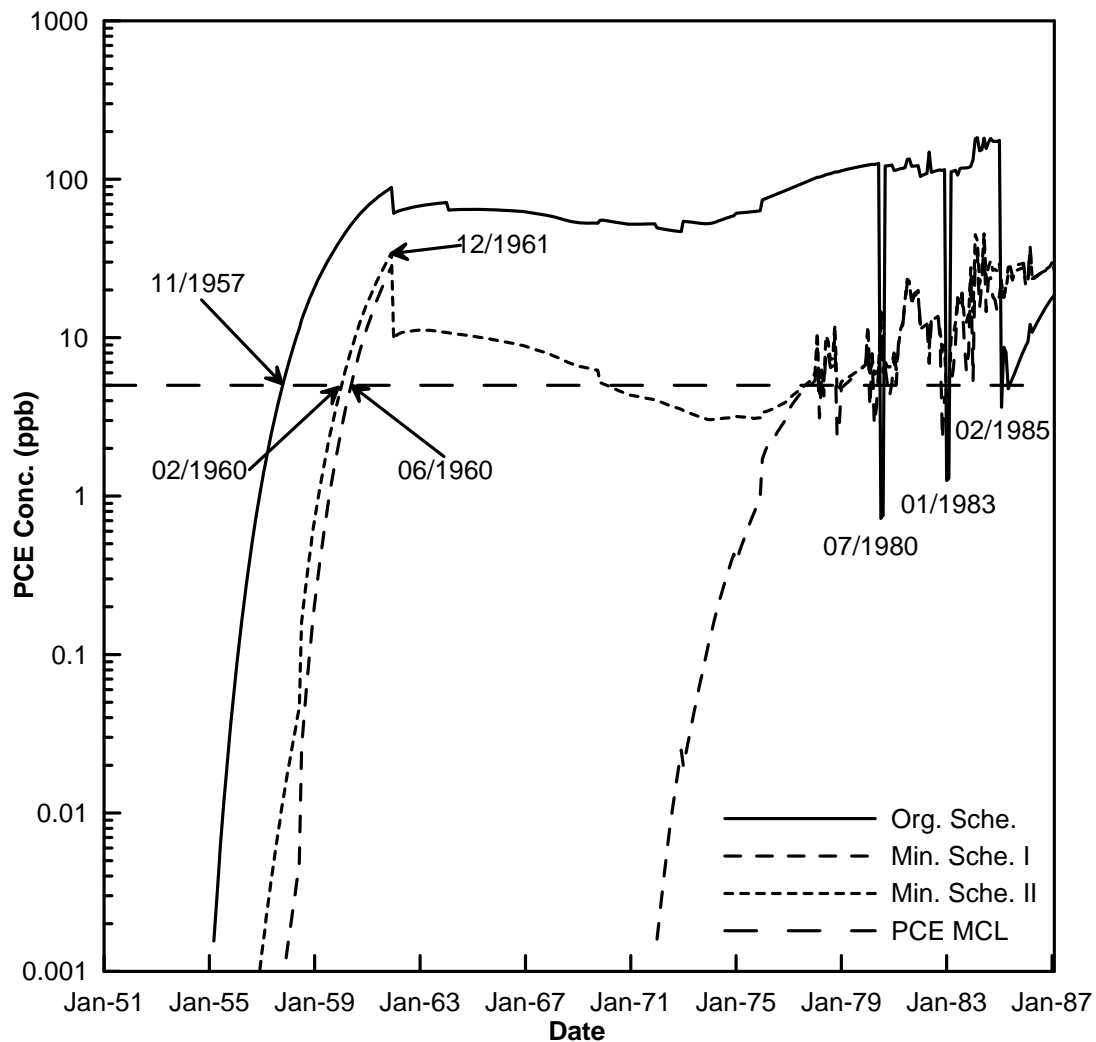


Figure 4.27. PCE concentrations in the WTP under the Original Schedule, the Minimum Schedule I, and the Minimum Schedule II

Based on the results presented in Figures 4.27 and 4.28 the following observations can be made:

- i. PCE concentration in the Tarawa Terrace WTP under the Minimum Schedule II is lower than that obtained under the Original Schedule except for the period after February 1985, which is similar to the Minimum Schedule I results;
- ii. PCE concentration in the WTP reached 5 ppb during February 1960 under the Minimum Schedule II, which is four months earlier than that obtained under the Minimum Schedule I and 27 months delayed when compared to the Original Schedule (November 1957);
- iii. Before January 1978, PCE concentration in the WTP under the Minimum Schedule II is higher than that obtained under the Minimum Schedule I, but the difference becomes very small after that time. This is because the pumping rate of well TT-26 under the Minimum Schedule II after January 1978 is quite

similar to that of the Minimum Schedule I;

- iv. Due to the continuous pumping schedule of well TT-26 under the Minimum Schedule II, the PCE concentration in the WTP does not decrease below 1 ppb as was observed under the Minimum Schedule I. In fact, PCE concentrations in the WTP were above 5 ppb most of the time after exceeding the MCL in February 1960, except for the period March 1970 through September 1977.

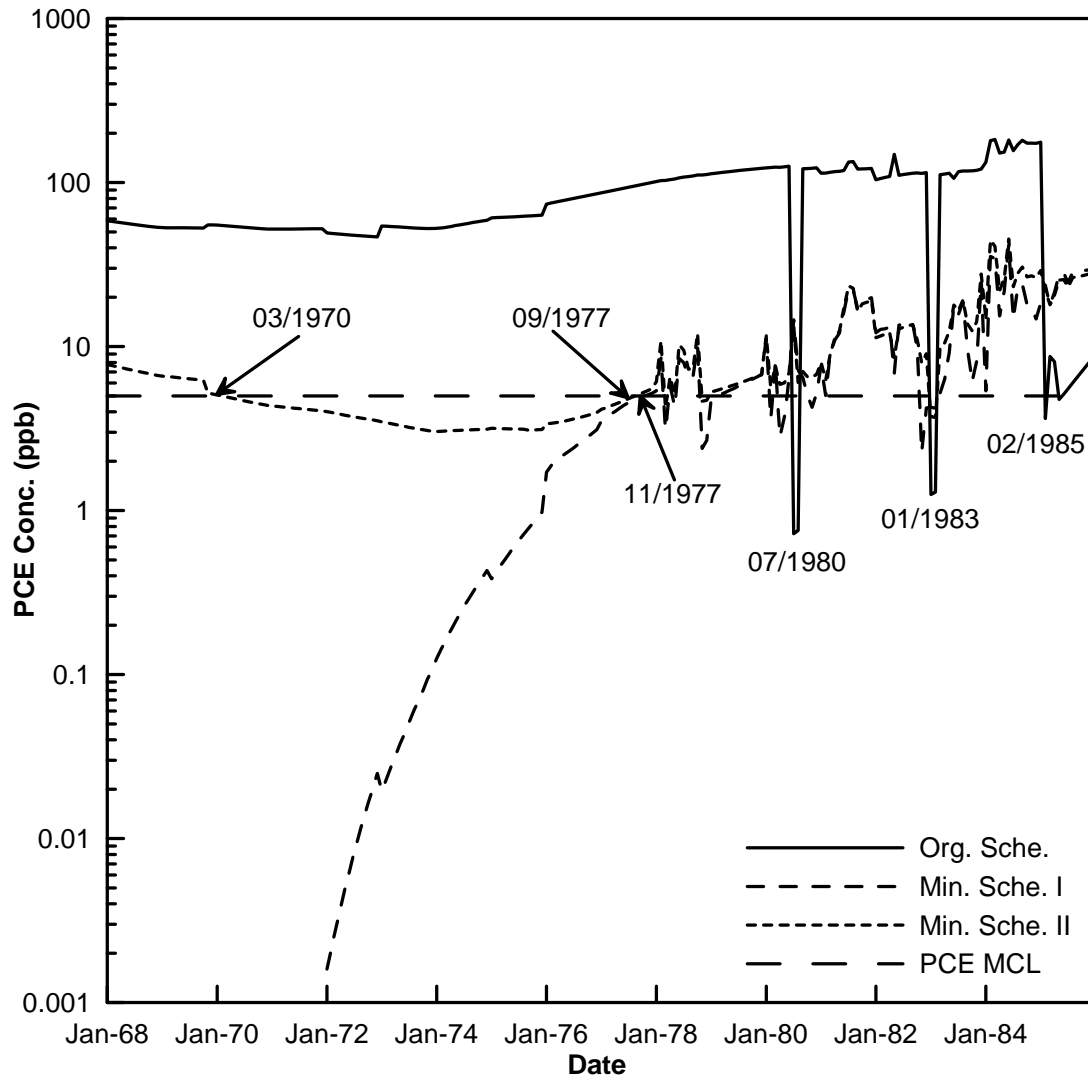


Figure 4.28. PCE concentrations in the WTP under the Original Schedule, the Minimum Schedule I, and the Minimum Schedule II for the period of interest

Similar to the results summarized in Tables 4.4 and 4.5, the total mass of contaminant withdrawn from the groundwater system by the water-supply wells under different pumping schedules is given in Table 4.6, and the PCE concentrations in the WTP are compared in Table 4.7. Based on the results given in Tables 4.6 and 4.7, one may conclude that by forcing the pumping rate of well TT-26 to be at least 25% of its pumping capacity throughout the simulation period, when compared to the Minimum

Schedule I, about 72% more PCE mass is withdrawn by pumping wells under the Minimum Schedule II, and the average PCE concentration in the WTP for the period of interest is approximately 60% higher.

Table 4.6. PCE masses withdrawn under the Original Schedule, the Minimum Schedule I, and the Minimum Schedule II

	Total Mass Released (g)	Mass Withdrawn (g)	Percentage (%)
Orig. Sche.	1.40×10^7	2.45×10^6	17.50
Min. Sche. I	1.40×10^7	1.98×10^5	1.41
Min. Sche. II	1.40×10^7	3.41×10^5	2.44

Table 4.7. PCE concentrations in the WTP under the Original Schedule, the Minimum Schedule I and the Minimum Schedule II for the period of interest* (Units: ppb)

	Maximum	Minimum	Average
Orig. Sche.	183.04	46.69	86.39
Min. Sche. I	41.36	7.84×10^{-8}	5.01
Min. Sche. II	45.31	3.04	8.04

* Data for July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985 are not included.

4.4 Summary of simulation results

4.4.1 Pumping rate in well TT-26

Based on the results summarized in previous sections, it may be concluded that the pumping schedule variation causes significant changes in the contaminant concentrations and MCL arrival times at both the water-supply wells and the WTP. In this case, the pumping rate in well TT-26 is critical to the PCE MCL arrival time because of its proximity to the contaminant source. The change of pumping rate in well TT-26 can cause PCE concentration in the WTP to change from trace levels to amounts several orders of times higher than the MCL. The pumping rate percentage in well TT-26 relative to its pumping capacity under different pumping schedules is summarized in Figure 4.29. Figure 4.30 is plotted to give a clear view of the variation of the pumping rate in well TT-26 between 1976 and 1985.

Based on the results given in Figures 4.29 and 4.30, the period January 1962 – February 1976 is when the pumping rate in well TT-26 could have varied the most. This period also is consistent with the most variation that is observed on the PCE concentrations in the water-supply wells and the Tarawa Terrace WTP under different pumping schedules. The periods when well TT-26 was out of service are consistent with the sudden drops of PCE concentration observed in the WTP under the Original Schedule and the Maximum Schedule.

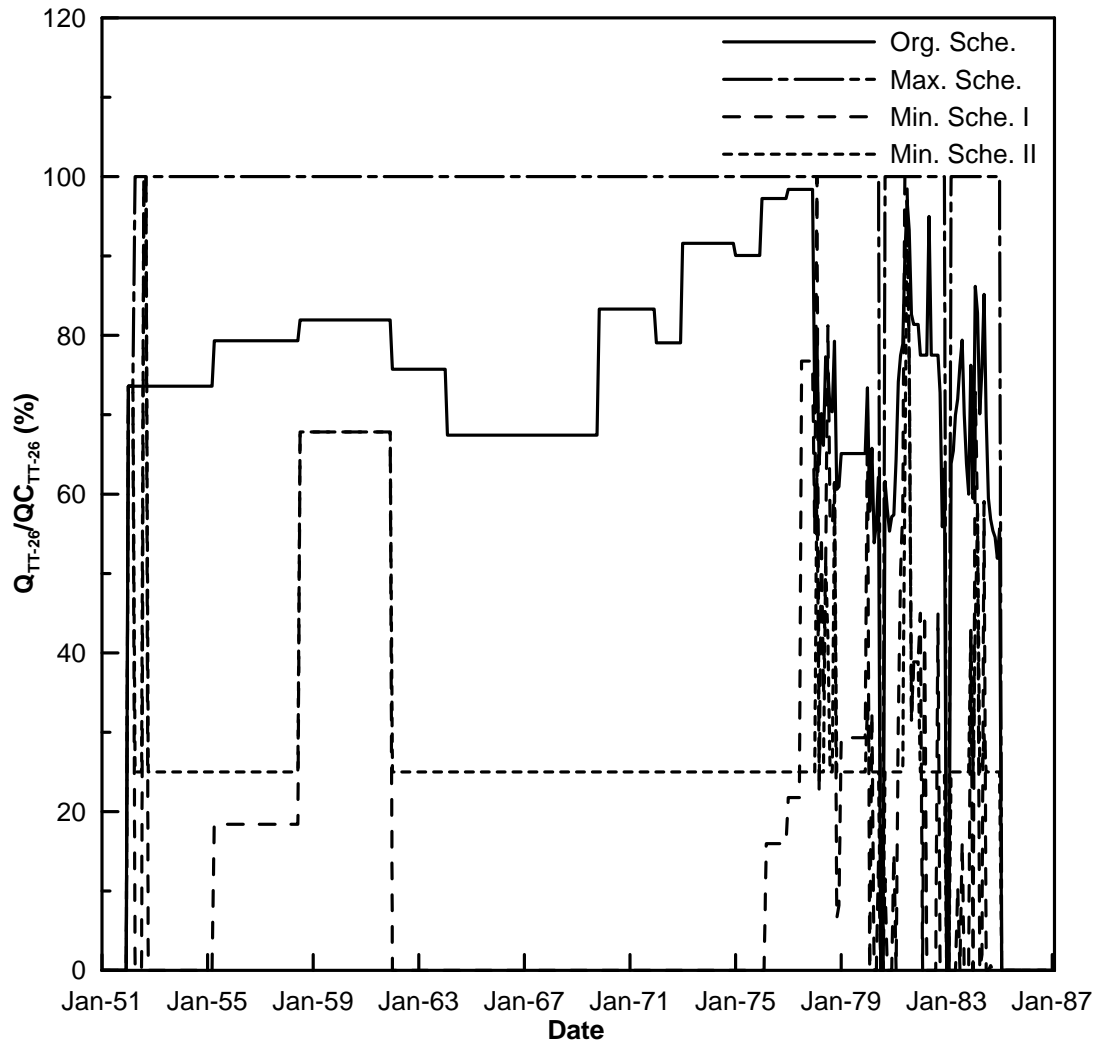


Figure 4.29. Percentage of pumping rate relative to its pumping capacity in well TT-26 under the Original and the updated pumping schedules

From the results presented in Figures 4.29 and 4.30, except for the first few months when pumping schedule has no significant effect on the PCE concentration, well TT-26 was always being operated at its full capacity for early arrival simulations. Under the Maximum Schedule, the PCE concentration in well TT-26 is always much higher than in the other water-supply wells. Therefore, the operation of well TT-26 at its capacity is required to obtain the maximum PCE concentration and the earliest arrival of PCE at the WTP. Under the two “late” arrival schedules, however, TT-26 was not pumping at the lowest possible rates for some stress periods near the end of the simulation. This occurs because in the second half of the simulation period for the “late arrival” cases, the PCE concentration in well TT-26 is no longer the dominant source of contaminants.

Again, all simulation results discussed here are based on the pumping capacities constructed for this study, which limits the maximum allowances for the changes in pumping rates. If this limiting factor is not considered, the pumping rates in the

water-supply wells may be changed without restriction, thus significantly affecting the PCE concentrations and MCL arrival times. However, this would not be a realistic solution.

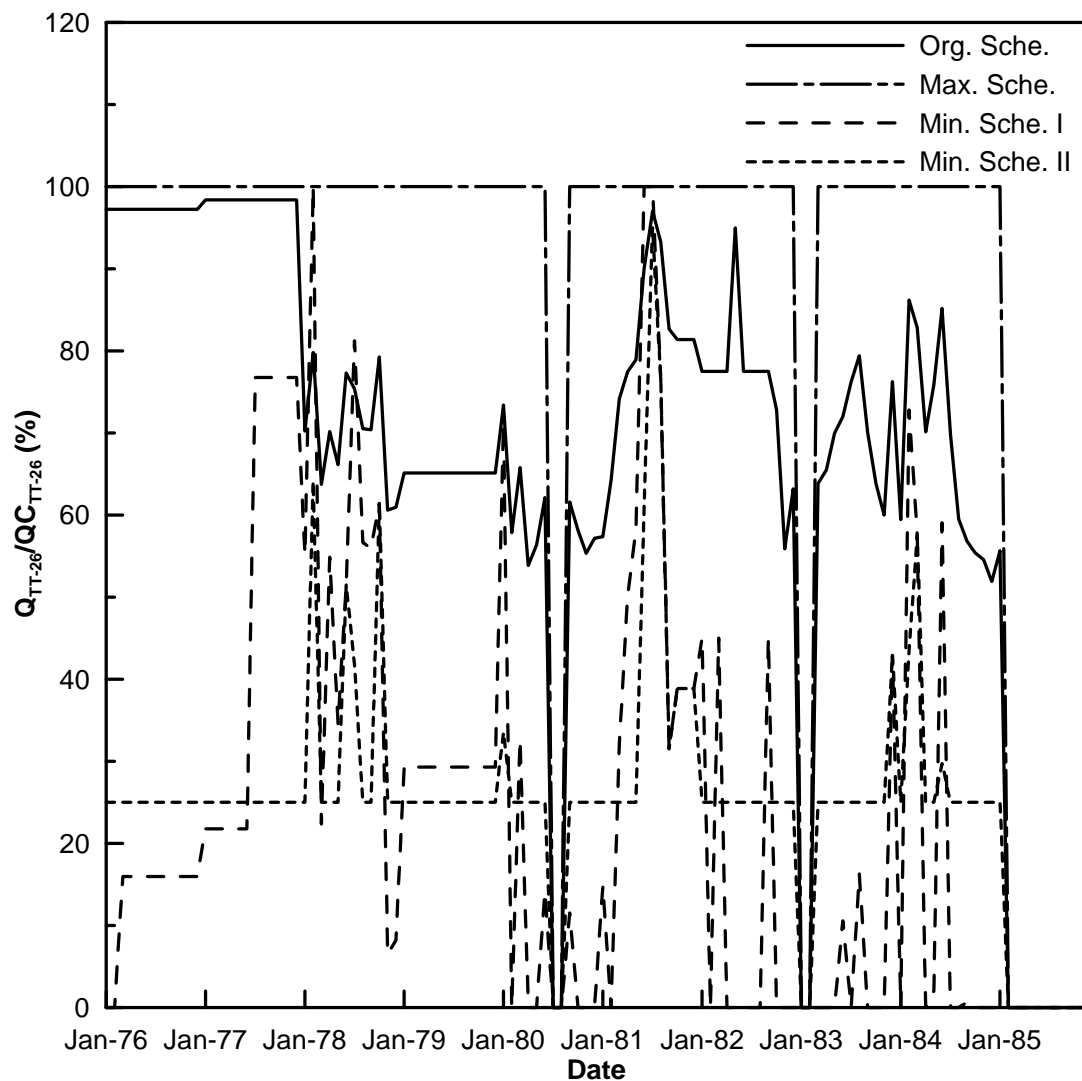


Figure 4.30. Percentage of pumping rate relative to its pumping capacity in well TT-26 under the Original and updated pumping schedules for the period of 1976 – 1985

4.4.2 PCE concentration in well TT-26

Simulation results for all three pumping schedules show that these schedules can cause changes in the PCE distribution in the groundwater system, in the PCE concentrations in the water-supply wells and the WTP, and in the PCE MCL arrival times. The comparison of PCE concentrations in water-supply well TT-26 under different pumping schedules is shown in Figure 4.31.

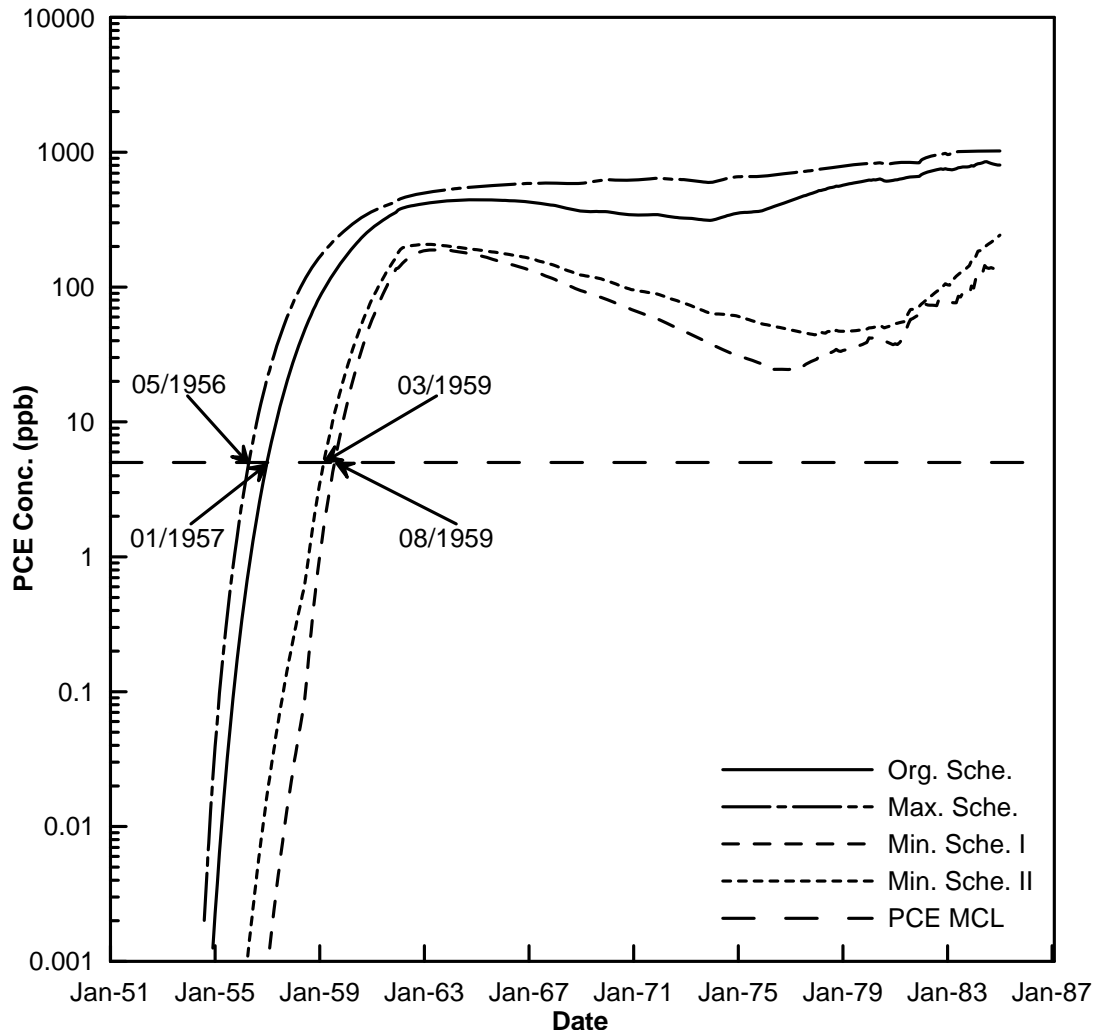


Figure 4.31. PCE concentrations in well TT-26 under the Original and updated pumping schedules

From the results shown in Figure 4.31, it can be concluded that the earliest time for PCE concentration in well TT-26 to reach the 5 ppb MCL is May 1956, and the latest date is August 1959. This indicates that given the hydrogeologic data together with, and only with, a change of pumping schedules, the 5 ppb arrival time of PCE in well TT-26 can vary from May 1956 to August 1959. This shows a 39-month variability between the “early” and “late” arrival dates. In this figure, the difference observed in the PCE MCL arrival time under the Minimum Schedule I is larger than the one observed under the Maximum Schedule relative to the Original Schedule results. The reason for this is, as shown in Figure 4.29, the change of pumping rate in well TT-26 in the first half of simulation period under the Minimum Schedule I is larger than the one under the Maximum Schedule, and the larger difference yields a more dispersed contaminant plume and a much lower PCE concentration in well TT-26. A comparison of PCE concentrations in well TT-26 is given in Table 4.8 for different schedules. PCE MCL arrival time in well TT-26 under different pumping schedules is given in Table 4.9.

Table 4.8. PCE concentrations in well TT-26 under the Original and updated pumping schedules for the period of interest* (Units: ppb)

Pumping Schedule	Maximum	Minimum	Average
Org. Sche.	851.19	312.62	490.62
Max. Sche.	1023.32	585.98	738.40
Min. Sche. I	144.74	24.49	58.28
Min. Sche. II	243.00	44.32	85.49

* Data for July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985 are not included.

Table 4.9. PCE MCL arrival times in well TT-26 under the Original and the updated pumping schedules

Pumping Schedule	Date
Org. Sche.	01/1957
Max. Sche.	05/1956
Min. Sche. I	08/1959
Min. Sche. II	03/1959

4.4.3 PCE concentration in the WTP

The PCE concentrations in the Tarawa Terrace WTP calculated from different pumping schedules are compared in Figures 4.32 and 4.33. Figure 4.32 shows the PCE concentration in the WTP during the period January 1951 – February 1987, while Figure 4.33 shows only the comparison of PCE concentrations in the WTP during the period of interest.

Results shown in Figure 4.32 indicate that the PCE concentration in the Tarawa Terrace WTP could reach the 5 ppb MCL as early as December 1956, or as late as June 1960. Compared to the PCE MCL arrival time in the WTP under the Original Schedule (November 1957), the PCE concentration in the WTP could reach the MCL 11 months earlier, or 31 months later.

These results are obtained without changing the other parameters that may affect the fate-and-transport of PCE in the subsurface and thus the 5 ppb PCE MCL arrival time in the WTP. Therefore, the variation of pumping schedule has an important effect on the PCE concentration in the Tarawa Terrace WTP and thus the MCL arrival time. A summary of the PCE concentration and MCL arrival time in the WTP under different pumping schedules can be seen in Tables 4.10 and 4.11.

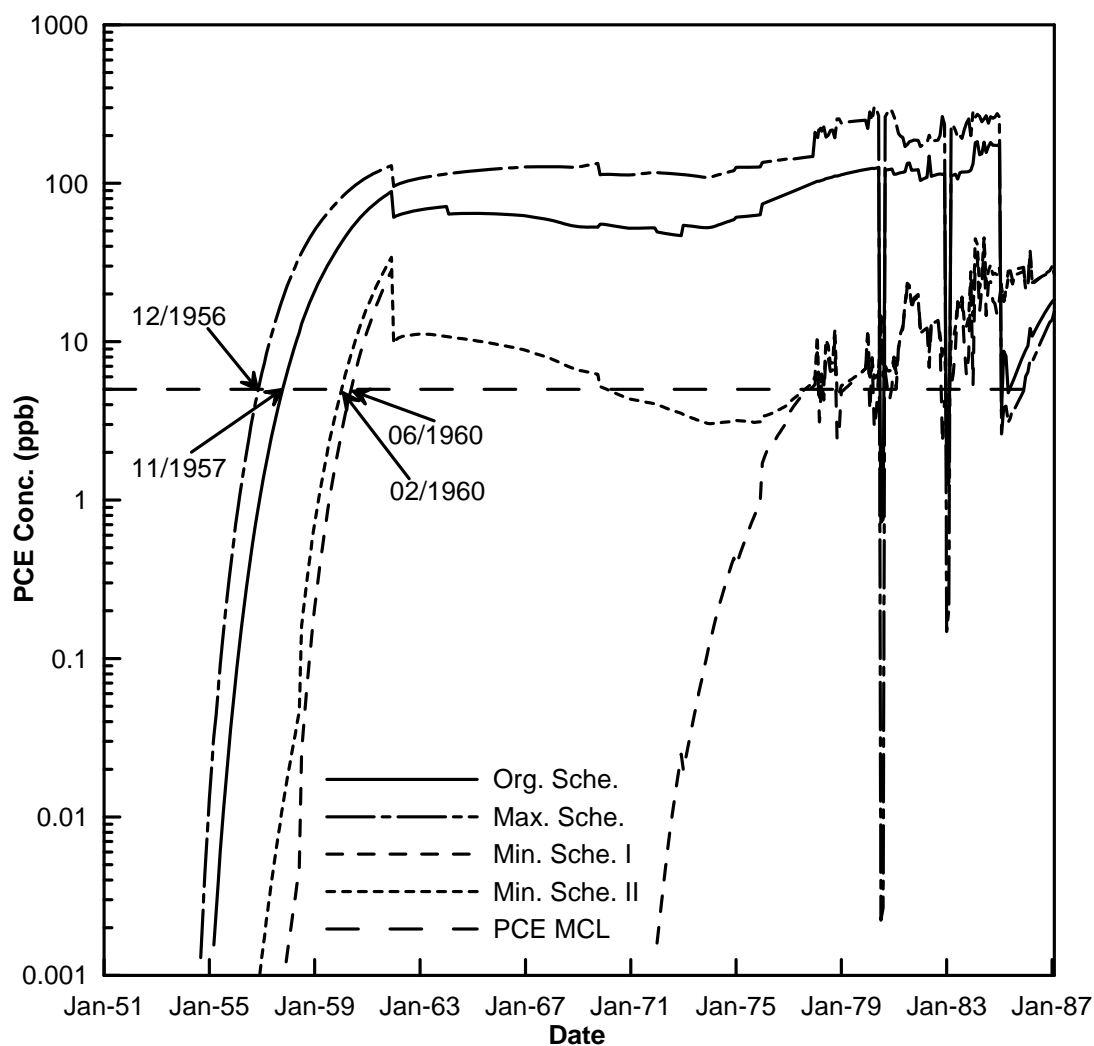


Figure 4.32. PCE concentrations in the WTP under the Original and the updated pumping schedules

Table 4.10. PCE concentrations in the WTP under the original and the updated pumping schedules for the period of interest* (Units: ppb)

Pumping Schedule	Maximum	Minimum	Average
Org. Sche.	183.04	46.69	86.39
Max. Sche.	304.66	108.76	166.07
Min. Sche. I	41.36	7.84×10^{-8}	5.01
Min. Sche. II	45.31	3.04	8.04

* Data for July 1980 – August 1980, January 1983 – February 1983, and February 1985 – December 1985 are not included.

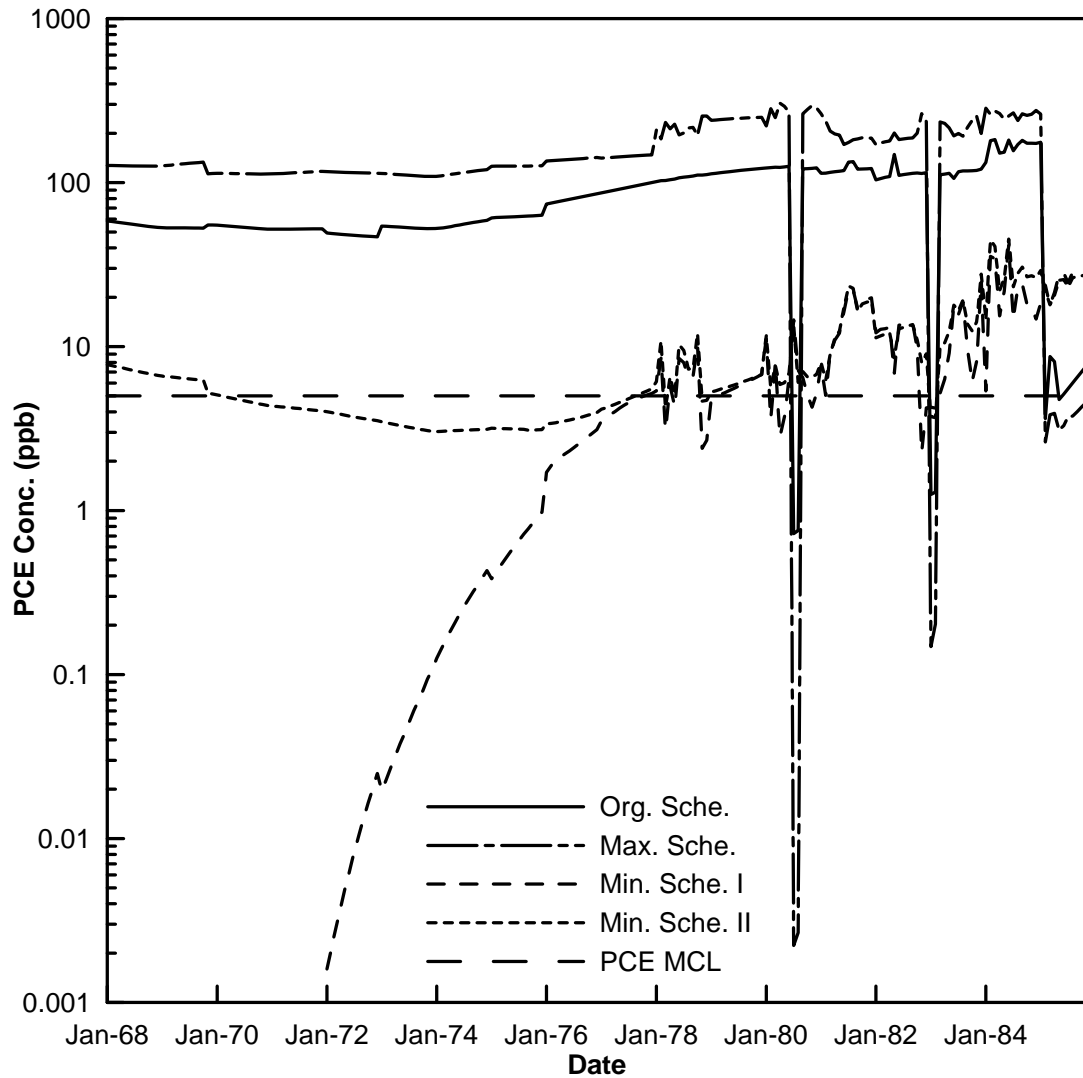


Figure 4.33. PCE concentrations in the WTP under the Original and the updated pumping schedules for the period of interest

Table 4.11. PCE MCL arrival times in the WTP under the Original and the updated pumping schedules

Pumping Schedule	Date
Org. Sche.	11/1957
Max. Sche.	12/1956
Min. Sche. I	06/1960
Min. Sche. II	02/1960

Variation of pumping schedules also changes the amount of contaminant mass withdrawn from the groundwater system. A summary of PCE masses withdrawn under different schedules is given in Table 4.12. In this table the change of mass withdrawn from the groundwater system is quite significant.

Table 4.12. PCE masses withdrawn under the Original and the updated pumping schedules

	Total Mass Released (g)	Mass Withdrawn (g)	Percentage (%)
Orig. Sche.	1.40×10^7	2.45×10^6	17.50
Max. Sche.	1.40×10^7	4.59×10^6	32.78
Min. Sche. I	1.40×10^7	1.98×10^5	1.41
Min. Sche. II	1.40×10^7	3.41×10^5	2.44

4.5 Conclusions

In this study, effect of pumping schedule variations on the PCE arrival times at the water-supply wells and the Tarawa Terrace WTP is evaluated. Because of the large scale and complexity of the problem, a procedure identified as PSOpS, which is based on the simulation/optimization (S/O) approach, has been developed. PSOpS was applied to optimize the pumping schedules for evaluation of PCE MCL arrival time in the Tarawa Terrace WTP. Final results of this study indicate that PSOpS works well for this study in a computationally cost-efficient manner.

Simulation results presented in this study lead to the following conclusions:

- i. Variation of pumping schedule has an effect on contaminant arrival time at the water-supply wells. According to our study results, a change in pumping schedules can cause changes in the contaminant plume distribution and the orientation of the plume front in the groundwater system. These changes in the contaminant transport characteristics lead to a variation of contaminant concentrations in the water-supply wells, which is equivalent to the variation of contaminant arrival time at the water-supply wells. For example, according to the results presented in this study, the arrival time of 5 ppb PCE concentration in well TT-26 varies from May 1956 to August 1959;
- ii. Variation of pumping schedules has an impact on the contaminant arrival time at the WTP, and this impact is twofold. The mixing model equation indicates that the PCE concentration in the WTP is calculated from the PCE concentrations and the pumping rates in the water-supply wells. Therefore, a variation of pumping schedule changes the contaminant arrival time at the WTP by affecting both of the factors of the mixing model equation. Simulation results reported in this study indicate that the PCE MCL arrival time in the Tarawa Terrace WTP varies from December 1956 to June 1960. This outcome is based on the allowable changes of the pumping schedules within the pumping capacity of each well;
- iii. Water-supply well TT-26 is critical in assessing the contaminant arrival time at the Tarawa Terrace WTP. All simulation results show that by the time the PCE concentration in the WTP reached 5 ppb, the PCE concentrations in all the water-supply wells, except well TT-26, were still negligible. This is due to some unique characteristics of well TT-26. First, well TT-26 is the closest water-supply

well to the contaminant source, the ABC One-Hour Cleaners. Second, well TT-26 is located in the downstream groundwater flow direction from the contaminant source. Finally, well TT-26 has the longest pumping history among all the water-supply wells. Therefore, increasing the pumping rate in well TT-26 can cause earlier contaminant arrival time at the WTP, and vice versa;

- iv. Variation of pumping schedules can cause a significant change in the amount of contaminant mass withdrawn from the groundwater system. Considering the total amount of water supplied to the WTP, a change in the PCE concentration in the WTP caused by a variation in the pumping schedules leads to the change in contaminant mass withdrawn. Given different pumping schedules derived in this study, the total PCE mass that was supplied to the WTP could vary from 1.41% to 32.78% of the total contaminant mass released from the contaminant source into the groundwater system at the site.

5 Summary of Results

In this study, changes in PCE concentrations and PCE MCL arrival times at the water-supply wells and the Tarawa Terrace WTP that could be initiated by a variation in pumping schedules has been analyzed. Considering the large scale and complexity of the problem, in an effort to find a solution within the time limits of the project and the computational power available, the following have been introduced to reduce the problem to a manageable level:

- i. The optimization problem has been reformulated so that the pumping schedules can be sequentially optimized based on the optimal solutions obtained from the previous stress periods; and,
- ii. An optimization technique identified as the rank-and-assign method has been developed to be used together with the improved gradient method for the solution of the optimization problem. Application of these two techniques reduces the number of iterations and the dimension of the problem, thus reducing the computational demand.

A three-dimensional contaminant transport simulation and an optimization model identified as PSOpS was developed based on the optimization techniques introduced above. PSOpS couples the groundwater flow and contaminant fate-and-transport simulation models, MODFLOW and MT3DMS, with the optimization techniques to optimize the pumping schedules to determine the early and late arrival times of contaminants at the site. Simulation results indicate that PSOpS works efficiently for the problem considered in this study.

Based on the optimal pumping schedules obtained from PSOpS, simulations have been conducted to demonstrate the effect of the pumping schedule variation on the PCE arrival times in the water-supply wells and the Tarawa Terrace WTP. Analyses of the simulation results indicate that a variation in pumping schedules can affect the PCE arrival time. Considering this uncertainty factor, a change of pumping schedules yields the following outcomes. According to the simulation results, the PCE MCL arrival time in well TT-26 would vary from May 1956 to August 1959, while the PCE MCL arrival time in the Tarawa Terrace WTP would vary from December 1956 to June 1960.

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