OPTIMAL STORAGE OF FRESHWATER IN SALINE AQUIFERS

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M. DENİZ KÜSTÜ

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Approval of the Graduate School of Natural and Applied Science.

Prof. Dr. Canan ÖZGEN
Director

I certify that this thesis satisfies all the requirements as a thesis for the degree of Master of Science.

Prof. Dr. Asuman G. TÜRKMENOĞLU
Head of Department

This is to certify that we have read this thesis and that in our opinion it is fully adequate, in scope and quality, as a thesis for the degree of Master of Science.

Prof. Dr. Hasan YAZICIGİL
Supervisor

Examining Committee Members

Prof. Dr. Ruşen GEÇİT (METU, ES)

Prof. Dr. Hasan YAZICIGİL (METU, GEOE)

Prof. Dr. Nurkan KARAHANOĞLU (METU, GEOE)

Assoc. Prof. Dr. M. Zeki ÇAMUR (METU, GEOE)

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Name, Last name: M. Deniz Küstü

Signature :

ABSTRACT

OPTIMAL STORAGE OF FRESHWATER IN SALINE AQUIFERS

Küstü, M. Deniz
M. S., Department of Geological Engineering
Supervisor : Prof. Dr. Hasan Yazıcıgil

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Storage of freshwater in saline aquifers has a strategic importance in water deficit countries. The freshwater stored in these aquifers may be the only source of water available during times of crisis. Coupled simulation and optimization type groundwater management models have been developed that will achieve the optimal control of the storage of freshwater in a stagnant manner for constant density and variable density flows in hypothetical single- and multi-layered saline aquifers.

The study is carried out in two stages. In the first stage, a transient model of five years is simulated that allows sufficient time for the freshwater mound to be created. In the second stage, an optimization model is formulated which minimizes the pumping/injection rates of a set of hydraulic gradient control wells subject to a set of constraints consisting of systems response equations, demand requirements, hydraulic gradient controls, pumping and injection limitations. The optimization models select which wells to be pumped and which ones to be injected and decide on their pumping/injection schedules to maintain the freshwater mound from migration. The results of the optimization models showed that the mound is successfully contained in its original location by controlling the hydraulic gradient via pumping/injection wells.

Keywords: Storage, freshwater, simulation, optimization, saline aquifer, variable-density flow

ÖZ

TUZLU SU AKİFERLERİNDE TAZE SU DEPOLANMASI

Küstü, M. Deniz
Yüksek Lisans, Jeoloji Mühendisliği Bölümü
Tez Yöneticisi: Prof. Dr. Hasan Yazıcıgil

Haziran 2005, 99 sayfa

Tuzlu su akiferlerinde taze su depolanması kurak ülkelerde stratejik açıdan önem taşımaktadır. Bu ülkelerde depolanan taze su, kriz zamanlarında mevcut olan tek su kaynağı olabilir. Hipotik tek ve çok katmanlı tuzlu akiferlerde, taze su depolanmasının optimal kontrolünün en iyi şekilde sağlanabilmesine yönelik sabit ve değişken yoğunluktaki akım için birleşik simülasyon ve optimizasyon tipi yeraltısuyu işletim modelleri geliştirilmiştir.

Bu çalışma iki kısımda yürütülmüştür. Birinci kısımda, taze su tümseğinin oluşumuna yetecek biçimde 5 yıllık zamana bağlı bir model simüle edilmiştir. İkinci kısımda ise; sistem tepki denklemlerini, su talebini, hidrolik eğim kontrollerini ve pompaj ve enjeksiyon sınırlarını içeren kısıtlamalar setine sahip olan ve hidrolik eğim kontrol setlerinin pompaj/enjeksiyon miktarını minimize eden bir optimizasyon modeli formüle edilmiştir. Bu optimizasyon modeli, taze su tümseğinin ilerlemesini önlemek amacıyla kuyuları pompaj ve enjeksiyon kuyusu olarak ayırmakta ve onların pompaj/enjeksiyon miktarlarını

belirlemektedir. Modellerin optimal çözümleri taze su tümseğinin, hidrolik eğimi kontrol eden pompaj ve enjeksiyon kuyuları aracılığıyla, başarılı bir şekilde orjinal yerinde tutulduğunu göstermiştir.

Anahtar Kelimeler: Depolama, taze su, simülasyon, optimizasyon, tuzlu su akiferi, değişken yoğunluktaki akım

TO MY FAMILY….

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CHAPTER 1

INTRODUCTION

1.1 Purpose and Scope

The inevitable growth of population and the foreseeable devastation of nature have caused a great demand of water all around the world giving rise to explore alternative methods to obtain and maintain freshwater. Accordingly, the concept of storing and containing freshwater in an optimal manner by using coupled simulation-optimization models is becoming a real-life issue, especially in arid regions where the aquifers are usually saline and the freshwater sources are limited. In these regions, the availability of freshwater becomes even less in times of crisis. Regarding this fact, storing freshwater into a saline aquifer would be strategically important, more than ever during drought or crisis times.

This study is carried out to demonstrate the storage and containment of a freshwater mound in a saline aquifer by using hydraulic gradient control wells operating at an optimal rate. For this purpose, a freshwater mound is created by injection wells in a hypothetical, saline confined aquifer. The freshwater mound is kept in its place by controlling the hydraulic gradient through the use of pumping and injection wells at the mound boundary while the groundwater is continuously being pumped from the other side of the aquifer for water supply purposes. A coupled simulation and optimization model which determines the best pumping/injection schedules is solved both for constant density and variable density cases in single- and multi-layered aquifers.

1.2 Procedure and Method

The procedure followed in this study is based on a coupled simulation and optimization modeling which achieves the optimal containment of a freshwater mound created in a confined aquifer system. Various aquifer types and flow conditions were examined in the problem. These cases involve the followings:

Case 1: Constant-density flow in a single-layered aquifer,
Case 2: Constant-density flow in a multi-layered aquifer,
Case 3: Variable-density flow in a single-layered aquifer,
Case 4: Variable density flow in a multi-layered aquifer.

Each aquifer system is solved separately in two stages. In the first stage, a transient simulation model of 5 years is built in order to allow sufficient time for the freshwater mound to be formed by using 3 freshwater injection wells while the aquifer is being constantly pumped on the down-gradient side to supply demand for public use by means of 3 pumping wells. The geometry of the freshwater mound is utilized to identify potential optimal well locations.

In the second stage, an optimization model is formulated which minimizes the pumping/injection rates of a set of hydraulic gradient control wells subject to a set of constraints consisting of systems response equations, demand requirements, hydraulic gradient controls, pumping and injection limitations. The optimization model selects which wells to be pumped and which ones to be injected and decides on their pumping/injection schedules to maintain the freshwater mound from migration.

CHAPTER 2

LITERATURE REVIEW

2.1 Groundwater Numerical Simulation Models

The movement of groundwater in the subsurface environment has become clear to visualize and understand with the use of groundwater models which are valuable tools that characterize a simplified version of the real system describing the subsurface conditions. Models provide useful information about the flow and transport processes in a groundwater system and help to develop a proper remedial strategy. They can also be used to understand the present behavior of the system and predict its future manners.

Among the various groundwater model types (i.e. *physical scale models* and *analog models*), *mathematical models* are the most useful ones. They are the representations of a flow system by a set of differential equations that can be solved either analytically or numerically. In order to develop a mathematical model, a conceptual understanding of the physical system to be modeled is necessary (Driscoll, 1986). Groundwater systems with simple boundary conditions and uniform parameters can be solved analytically by making assumptions that simplify the governing equations. However, the reliability of these models are quite low due to the simplifications. For this reason, more complex aquifer systems are solved by numerical techniques. Numerical models are especially useful for aquifers having irregular boundaries, complex structures and variable pumping or recharge rates (Mercer and Faust, 1981).

During the past decades, numerical simulation models which apply finite difference or finite element methods to groundwater flow equations have been well-developed and become very common tools for helping the groundwater managers in the interpretation and management of an aquifer system.

In a *finite difference* and/or *finite element* technique, the flow domain is discretized into elements to each of which the system parameters are assigned. The variables are given by a finite number of algebraic equations defining certain parameters like decision variables (e.g. pumpage) that provide a control over the state variables (e.g. drawdown or hydraulic head), and spatially distributed system parameters that define the conductivity (e.g. transmissivity) and storage properties (e.g. storativity) of the system. These continuous variables are replaced with a set of discrete points arranged in a grid pattern within the system domain (Fetter, 1994). The grid is interconnected with nodal points at which the unknown variables such as the hydraulic head or the concentration of a contaminant are solved. The grid can be arranged as a *block-centered* grid (i.e. node points are located in the center of each cell), or a *mesh-centered* grid (i.e. node points lie at the intersections of the grid lines) depending on the boundary conditions. The network of nodes created in a finite-difference method is regularly-shaped whereas the finite-element method utilizes polygonal cells which are especially helpful in simulating problems with a moving boundary. Among the various groundwater simulation models, the *modular three-dimensional finite difference flow model - MODFLOW* developed by McDonald and Harbaugh (1984) is the most well-known and the widely-used one.

The increase in the number of groundwater contamination problems has lead to a growing concern of how to manage and restore the contaminated areas. For this purpose numerous contaminant transport models have been developed using finite-difference and finite-element methods. However, building a flow and solute transport simulation model is not sufficient for determining the optimal operating policies for an aquifer system. Therefore, groundwater management models are improved by combining the simulation models with optimization methods. A combined model considers the particular behavior of a given groundwater system and determines the best operating policy under the objectives and restrictions dictated by the water manager (Gorelick, 1983). The combined model also enables to determine the trade-offs associated with the various system's objectives (Willis and Liu, 1984; Dauer et al., 1985; Yazıcıgil and Rasheeduddin, 1987; Yazıcıgil, 1990).

2.2 Groundwater Hydraulic Management Models

In the review paper of Gorelick (1983), the groundwater management models are classified into two classes such as *groundwater hydraulic management models* and *groundwater policy evaluation and allocation models*.

Groundwater policy evaluation and allocation models are used for complex problems in which the economic management objectives are of concern together with the hydraulic management targets. They are usually described by multiple optimizations having a strong economic management component.

The *groundwater hydraulic management models*, on the other hand, are developed by integrating a simulation model of a particular groundwater system as constraints acting to limit the objective function of the management model. Although, these models focus mainly on managing system stresses such as groundwater withdrawals and recharge rates, economic factors may be explicitly (i.e. well costs and net benefits) or implicitly (i.e. total pumpage rates or drawdown) included in the objective function of the management model.

Two methods are employed in the hydraulic management of a groundwater system. The first one is called the *embedding technique* which involves the addition of a numerical discretization of the partial differential equation of flow in the aquifer as an explicit set of constraints in the optimization model. This technique produces head solutions at every node of the grid of the aquifer. The second approach, called as *response matrix approach*, provides only a set of responses at specified observation locations due to a unit pumping at a well site. These responses are then assembled to create the response matrix to be incorporated into the management model. The embedding approach provides more detailed information whereas the response matrix approach gives information only at specified locations. However, the huge amount of information causes an increase in the problem size leading to unstable numerical solutions in the embedding approach. For this reason, applications of the embedding approach should be restricted to small-scale steady-state problems.

Both methods can be applied to different optimization techniques such as linear, mixed-integer or quadratic programming in combination with groundwater simulation models where the objective function aims at minimizing the costs or maximizing the well production subject to a set of linear constraints that determine the values of decision variables (i.e. drawdowns, hydraulic gradients or pumping and/or injection rates).

2.3 Response Function Approach

Response functions express the changes in an aquifer system (groundwater levels or stream and spring discharge) resulting from groundwater pumping or recharge at a specified site for a specified time duration (Johnson, 1998). Each response describes the influence of a unit pulse of pumpage or injection upon drawdown or build-up over space and time at specified observation locations in the system (Figure 2.1). They may be developed either analytically or numerically by using finite-difference or finite-element methods.

Response functions may be used to understand the pumping and recharge effects on an aquifer, to realize the impacts of pumping or recharge on the groundwater levels, or to generate a response matrix to be incorporated into optimization models. For a groundwater management problem involving a coupled simulation-optimization model, the development of response functions is essential in order to identify the character of the system and manage its requirements.

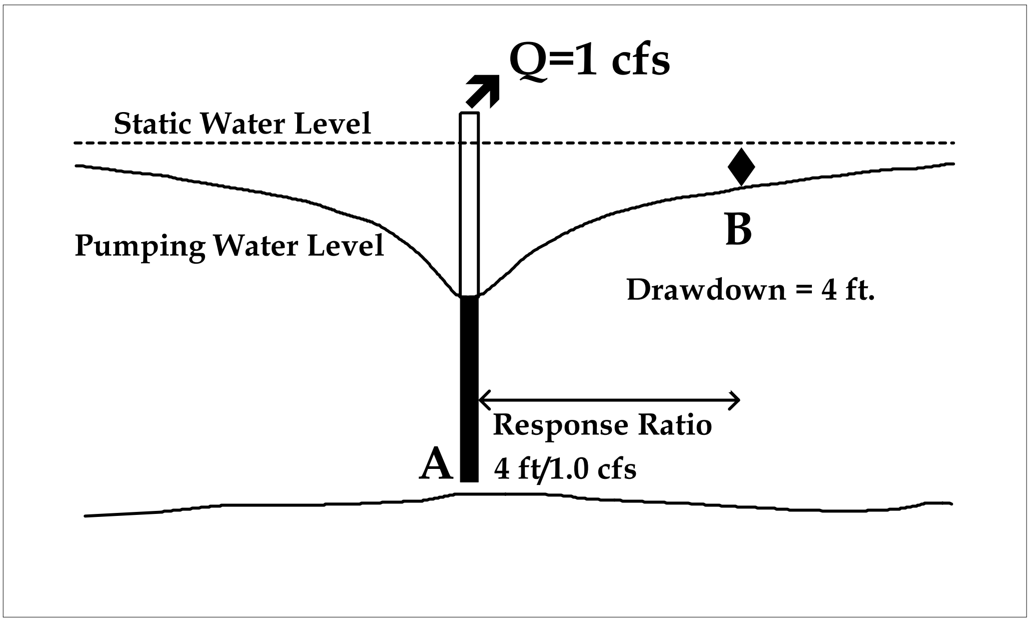


Fig. 2.1 A simplified diagram explaining the response function approach (Johnson, 1998).

The only restriction in the use of response functions is that they can only be applied to linear aquifer systems. If the responses generated within a system are non-linear, then the *principle of superposition*, which allows the responses to be superimposed or added to obtain the total system response at a particular point, can not be applied.

The response matrix approach has been widely applied to hydraulic management problems involving various objective functions such as the minimization of well costs and the maximization of well production (Lee and Aronofsky, 1958; Deninger, 1970; Wattenbarger, 1970; Maddock, 1972; Rosenwald and Green, 1974). All of the previous studies proved that the response matrix approach is an efficient way of evaluating management alternatives for complex aquifer systems.

2.4 Previous Studies

The optimal storage and containment of freshwater through the use of coupled simulation-optimization models have been studied by various researchers. The idea of storing freshwater into saline aquifers actually began in the late 1960's.

Esmail and Kimbler (1967) investigated the technical feasibility of storing freshwater in saline aquifers from a recovery viewpoint. Five hypothetical aquifers having different physical properties were constructed as laboratory models. They have also developed mathematical models showing the effects of dispersion and gravitational segregation on the recovery losses. The results showed that the storage of freshwater in saline aquifers is feasible under favorable conditions such as low permeabilities, high flow rates and short storage times.

Kimbler (1970) used laboratory flow models to verify the basic mechanisms that affect the recovery of freshwater stored in saline aquifers. The tests proved that the recovery efficiency is highly dependent on the physical and operating parameters of the system and increases as the rate of gravitational segregation decreases.

Moulder (1970) searched for the main factors affecting the recovery of freshwater stored in saline aquifers. He carried out in-situ injection and recovery tests which demonstrated that the freshwater recovery decreases as the time between injection and extraction (i.e. storage time) increases.

Molz and Bell (1977) controlled the head gradients in a storage area by installing an array of wells external to that area. They used the linear programming technique of Aguado and Remson (1974) to an artificially stored fluid body in order to achieve zero fluid displacement under steady-state conditions. The model results provided the minimum pumping and injection rates creating zero gradients in the storage area.

Atwood and Gorelick (1985) developed a two-stage planning procedure to stabilize and remove a groundwater contaminant plume by controlling the hydraulic gradient with a combined simulation-optimization model. In the first stage the flow and solute transport model is simulated and the contaminant plume geometry is determined. The second stage consists of the optimal well selection and pumping/recharge schedule determination by a linear program. Dividing the study into two stages eliminates the nonlinearities.

Aral (1989) demonstrated that the optimal hydraulic gradient control technique can be extended to multi-layer aquifers. The hydraulic stabilization of a contaminant plume in a multi-layered confined aquifer was achieved through the use of pumping and recharge wells at the bottom layer.

The effects of density on groundwater flow is a popular research area since the early 1970’s and is still driving the attention of many researchers. In many groundwater problems, the groundwater density varies as a function of the temperature and/or solid concentration of the fluid and affects the groundwater flow patterns. Field and laboratory studies have shown that fluid density gradients caused by variations in concentration and/or temperature can play an important role in the transport of solutes in groundwater systems involving groundwater contamination, seawater intrusion in coastal aquifers, radioactive waste disposal, geothermal energy development, groundwater–surface water interaction, and subsurface storage of materials, fluids, and energy (Simmons et al., 2001).

In order to simulate groundwater systems having significant density variations, numerical models simulating the density-dependent groundwater flow are developed. Among the various models, the most common and well-known one is called *SUTRA (Saturated–Unsaturated Transport),* which is a computer program for simulating density-dependent groundwater flow and solute transport (Voss, 1984). The model employs a 2-D/3-D finite-element and finite-difference method to approximate the governing equations that describe the saturated or unsaturated density-dependent groundwater flow and the transport of either thermal energy or dissolved substances in the subsurface environment (Voss and Provost, 2003).

Another numerical model used for simulating variable-density flow is called, the *USGS density-dependent groundwater flow and solute transport model, SEAWAT-2000* (Langevin et al., 2004). The SEAWAT-2000 code combines a modified version of MODFLOW-2000 (Harbaugh et al., 2000) and MT3DMS (*the multi-species transport model for saturated porous media* by Zheng and Wang, 1999) into a single computer program. The code was developed by reformulating the governing equation for variable-density groundwater flow in terms of equivalent freshwater head allowing constant density MODFLOW routines to solve for variable density groundwater flow with relatively few modifications (Langevin et al., 2004). SEAWAT-2000 enables the simulation of three-dimensional, variable-density, transient groundwater flow in porous media with or without simulating the solute transport. The *Variable-Density Process (VDF)* in SEAWAT-2000 uses equivalent freshwater head as the dependent variable in the variable-density groundwater flow equation. The utilization of equivalent freshwater head enables the use of MODFLOW structure and subroutines with little adjustments in order to solve the variable-density groundwater flow equation.

The numerical relation between the head and the equivalent freshwater head can be explained by the following equations (Guo and Langevin, 2002):

$$h_f = \frac{\rho}{\rho_f} h - \frac{\rho - \rho_f}{\rho_f} Z \tag{2.1}$$

$$h = \frac{\rho_f}{\rho} h_f + \frac{\rho - \rho_f}{\rho} Z \tag{2.2}$$

where ρ is the density of the native aquifer water (ML^{-3}), ρ_f is the density of freshwater (ML^{-3}),and Z is the elevation at the measurement point (L).

The governing equation for variable-density groundwater flow, in terms of equivalent freshwater head, is derived by Guo and Langevin (2002) as:

$$\begin{aligned} &\frac{\partial}{\partial \alpha}\left[\rho K_{f\alpha}\left(\frac{\partial h_f}{\partial \alpha} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \alpha}\right)\right] + \frac{\partial}{\partial \beta}\left[\rho K_{f\beta}\left(\frac{\partial h_f}{\partial \beta} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \beta}\right)\right] \\ &+ \frac{\partial}{\partial \gamma}\left[\rho K_{f\gamma}\left(\frac{\partial h_f}{\partial \gamma} + \frac{\rho - \rho_f}{\rho_f}\frac{\partial Z}{\partial \gamma}\right)\right] = \rho S_f \frac{\partial h_f}{\partial t} + \theta \frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t} - \rho_s q_s \end{aligned} \tag{2.3}$$

where α, β, and γ are orthogonal coordinate axes, aligned with the principal directions of permeability, K_f is equivalent freshwater hydraulic conductivity (LT^{-1}), S_f is equivalent freshwater specific storage (L^{-1}), t is time (T), θ is effective porosity (dimensionless), C is solute concentration (ML^{-3}), ρ_s is the fluid density source or sink water (ML^{-3}), and q_s is the volumetric flow rate of sources and sinks per unit volume of aquifer (T^{-1}).

Fluid density is assumed to be a function only of solute concentration for a coupled variable-density flow and solute-transport simulation. The following linear equation of state represents the fluid density as a function of solute concentration:

$$\rho = \rho_f + \frac{\partial \rho}{\partial C} C \tag{2.4}$$

CHAPTER 3

SIMULATION MODEL

The groundwater hydraulic management model for optimal containment of freshwater is applied to a hypothetical confined aquifer system which is shown in Figure 3.1. It is a standard simple groundwater system containing moderate saline water. In order to obtain reasonable and applicable results, the model parameters are selected consistently with the real world aquifer system parameters. The single and multi-layered constant-density cases are simulated by using the three-dimensional finite-difference groundwater flow simulation model of USGS, MODFLOW-2000 (Harbaugh et al., 2000) whereas the variable density single and multi layer cases are simulated by the USGS density-dependent groundwater flow and solute transport model, SEAWAT-2000 (Langevin et al., 2004).

The flow domain is discretized into uniform finite-difference cells each having a dimension of 200 x 200 m. The aquifer area is 200 km^2. The finite-difference mesh together with the well distribution is shown in Fig. 3.1.

To be able to observe the reversal of hydraulic gradients, the boundary conditions are chosen in such a way that they create a regional head difference from east to west. The eastern and western boundaries are defined as constant-head boundaries at 1000 meters above sea level (masl) and 900 masl, respectively, whereas the northern and southern boundaries are represented by no-flow boundaries (Fig. 3.1). For the variable-density cases, the eastern and western boundaries are assigned as constant-concentration boundaries having a value of 7000 mg L^{-1}.

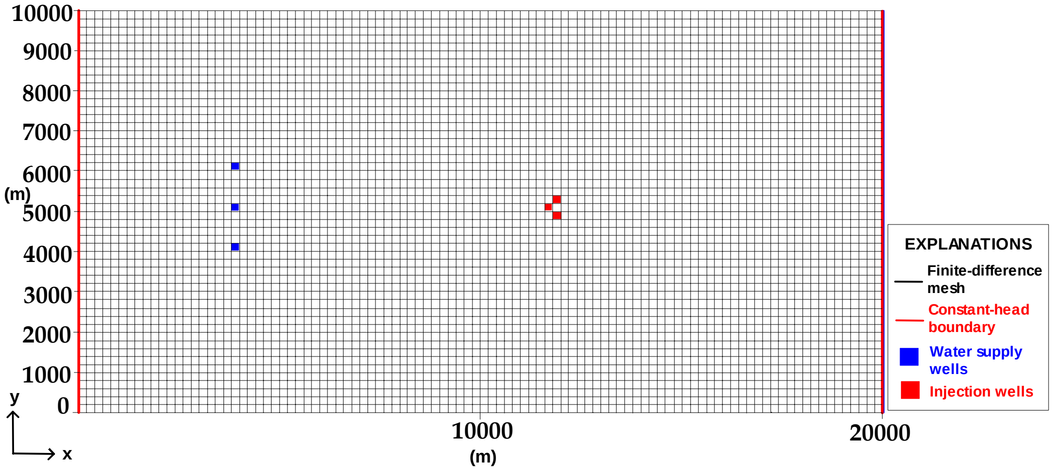


Fig. 3.1 Finite difference mesh and boundary conditions.

The aquifer is assumed to be a typical anisotropic homogeneous sandy aquifer. The hydraulic conductivity is assigned as 10 m day^{-1} in the x-direction and 5 m day^{-1} in the y-direction. The longitudinal and transverse dispersivities are assigned as 30 m and 3 m, respectively. The porosity is accepted as 0.2. A uniform specific storage value of $2*10^{-6}$ m^{-1} is assigned to each node in the finite difference mesh to characterize a confined flow. The native water salinity of the aquifer is assumed to be 7000 mg L^{-1} while the salinity of injected freshwater is taken as 500 mg L^{-1}. The aquifer thickness is set to a constant value of 50 m. For the multi-layered cases, the aquifer is separated into five individual layers, each having a constant value of 10 m.

The optimal capacity of freshwater storage and containment problem is applied under transient flow regimes. In order to conduct a transient run, the initial conditions of the system are needed. Thus, the initial head and concentration values of the system are obtained by simulating a steady-state run prior to injection and then the results of this steady-state run are used as the initial conditions for the transient simulation. This is accomplished by using the new capability of MODFLOW-2000 as setting the first stress period a steady-state stress period and making the rest of them transient stress periods. The simulation horizon of 5 years is divided into twenty one 3-month stress periods, which are further subdivided into 90 time steps to be able to obtain daily outputs. The problem is simulated by the PCG2 (*Preconditioned-Conjugate Gradient*) solver. Steady-state head distributions for the constant-density and the variable-density system are shown in Figures 3.2 and 3.3, respectively. After the steady-state head distribution of the system is obtained, the injection wells are activated to create the freshwater mound. The pumping wells kept on pumping with a rate of 15 L s^{-1} during the entire simulation time.

The well networks used for the creation of the freshwater mound in constant- and variable-density cases are also shown in Figures 3.4 and 3.5. Three freshwater injection wells are located in the eastern part of the aquifer while three pumping wells are placed on the western side of the aquifer. The mound is generated by injecting 10 L s^{-1} of freshwater into the aquifer from each of the three injection wells making a total of 30 L s^{-1}.

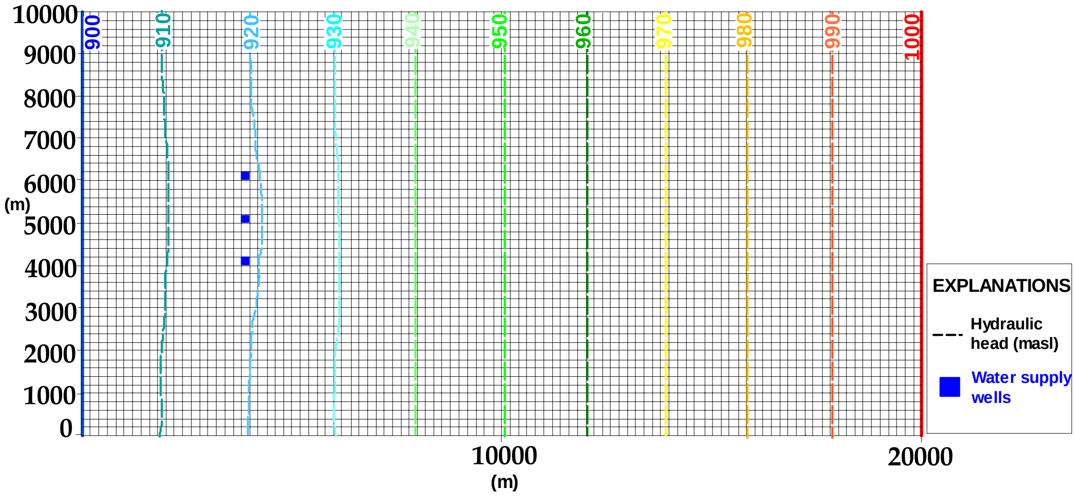


Fig. 3.2 Steady-state head distribution of the single- and multi-layered constant-density systems.

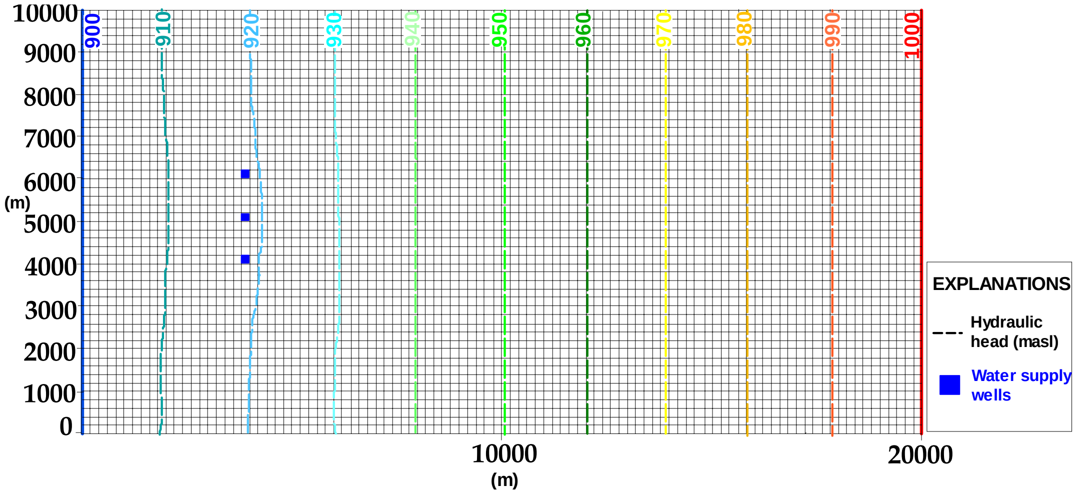


Fig. 3.3 Steady-state head distribution of the single- and multi-layered variable-density systems.

Figures 3.6 and 3.7 show the close-up views of the freshwater mound created at the end of five-year simulation time for the constant density and the variable-density cases, respectively. As it can easily be seen from the figures, the mounds are almost the same for both cases.

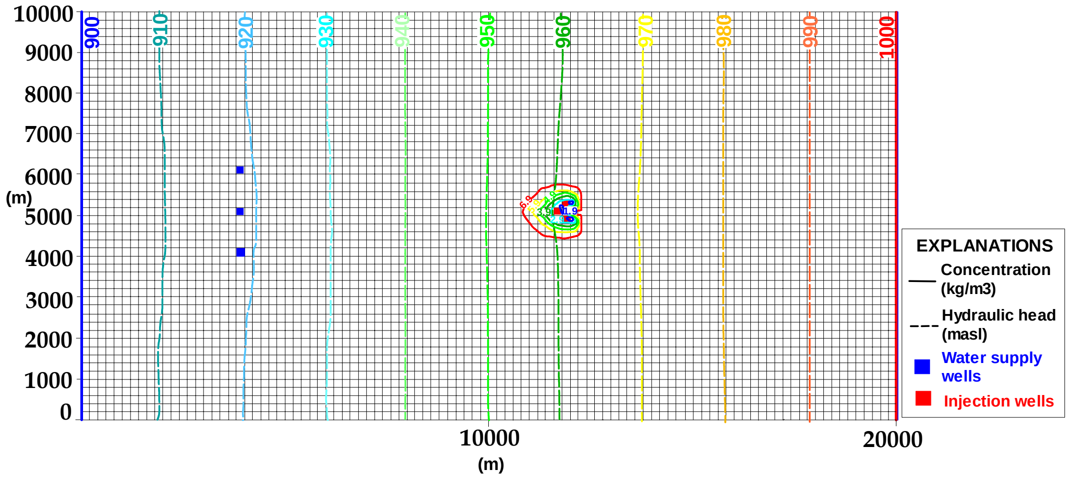


Fig. 3.4 Well distribution together with the freshwater mound created at the end of the simulation horizon for the single- and multi-layered constant-density cases.

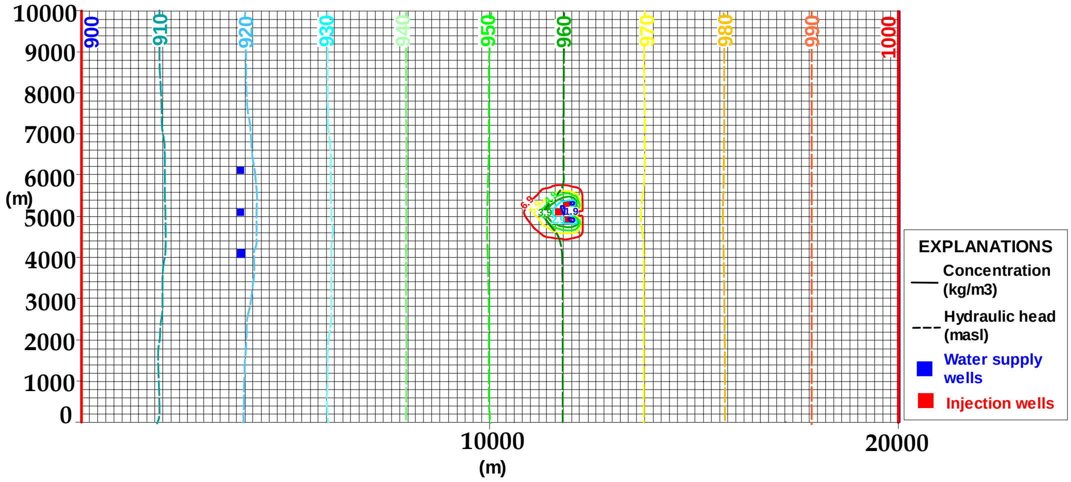


Fig. 3.5 Well distribution together with the freshwater mound created at the end of the simulation horizon for the single- and multi-layered variable density cases.

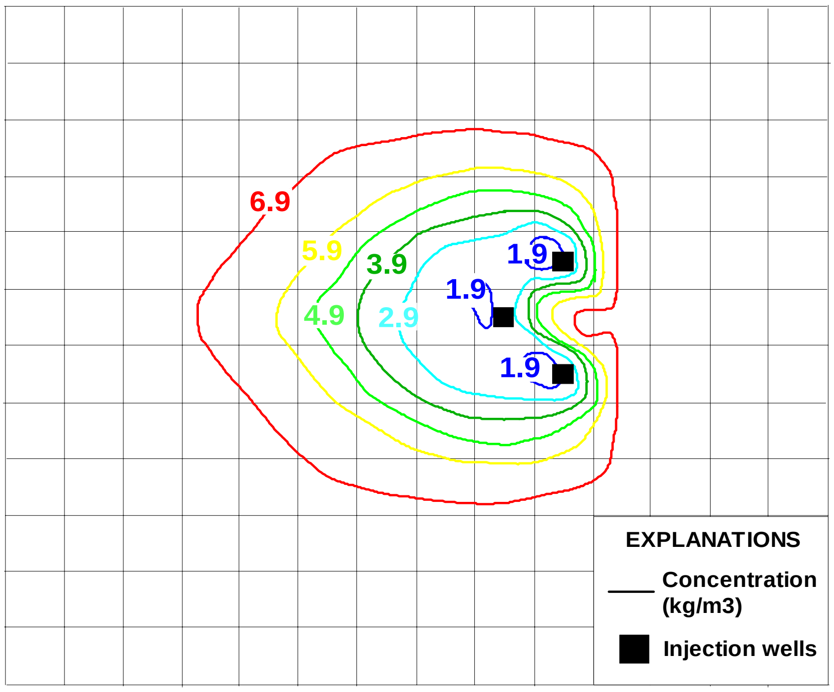


Fig. 3.6 Close-up view of the freshwater mound created at the end of the simulation horizon for the single- and multi-layered constant-density case.

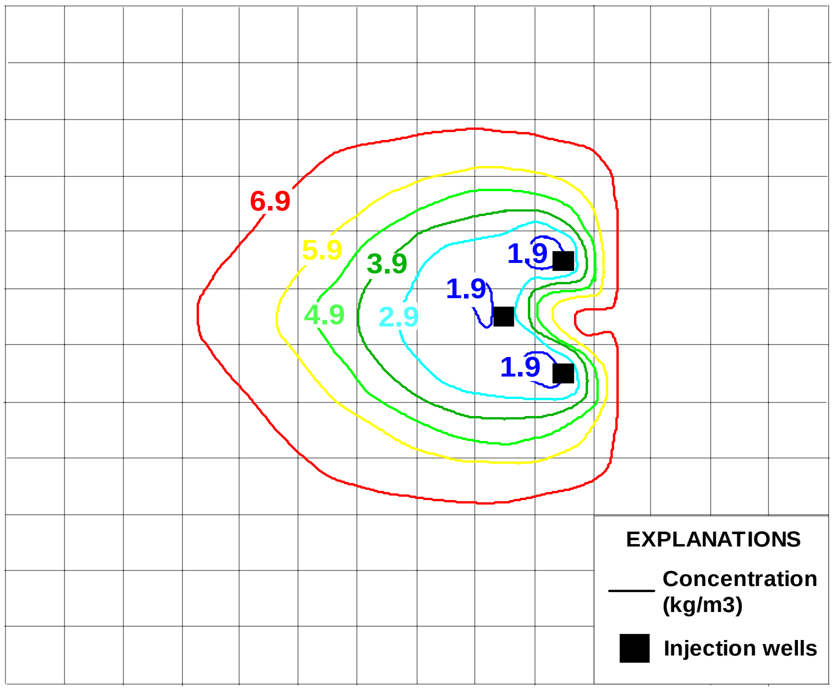


Fig. 3.7 Close-up view of the freshwater mound created at the end of the simulation horizon for the single- and multi-layered variable-density case.

For the solute-transport part of the simulation model, advective mechanisms are assumed to be dominant in the aquifer system to be able to develop a linear simulation management model. The *third-order TVD (ULTIMATE)* scheme is utilized for the advective transport solution of the model. The ULTIMATE algorithm *(Universal Limiter for Transient Interpolation Modeling of the Advective Transport Equations)* belongs to the class of transport solution techniques called as the *total-variation-diminishing (TVD)* methods which are designed for solving advection-dominated transport problems. The third-order ULTIMATE scheme is mass conservative, without excessive numerical dispersion and essentially oscillation-free (Zheng and Wang, 1999).

CHAPTER 4

RESPONSE MATRIX

A linear programming model combined with groundwater flow simulation is formulated by using the response function approach which describes the influence of a unit pulse of pumpage or injection upon drawdown or build-up over space and time at specified observation locations. Response functions are based on the linear systems theory enabling the use of the principle of superposition which is the process of combining the individual solutions. In the response matrix technique, the influences obtained by imposing a unit stress at a specified location are incorporated into constraints of the optimization model. A unit stress is a pulse source which has a fixed constant value for a specified period and has a zero value thereafter (Gorelick et al., 1993).

Maddock (1972) has shown the discrete form of the drawdown response function for a linear flow system as:

$$s(k,n) = \sum_{j=1}^{M} \sum_{i=1}^{n} \beta(k, j, n - i + 1) Q(j,i) \tag{4.1}$$

where $s(k,n)$ = drawdown at pumping well k at the end of planning period n (L), $\beta(k, j, n - 1 + 1)$ = drawdown response function at the kth well at the end of nth period due to a unit pumping at the jth well applied throughout the ith pumping period ($T\ L^{-2}$), $Q(j,i)$ is the average volumetric discharge rate at pumping well j during pumping period i ($L^3\ T^{-1}$), M is the total number of water supply wells and injection/pumping wells (which will be called as containment wells hereafter), and N is the total number of planning periods.

The response functions in this study are created by running multiple transient simulations of the finite-difference model MODFLOW-2000 for the constant-density cases and SEAWAT-2000 for the variable-density cases. The response equations generated for this study include two kinds of responses; drawdown responses for the pumping wells and build-up responses for the injection wells. The coefficients of the response matrix are created by assigning a unit discharge and recharge of 1 $m^3 s^{-1}$ at the first stress period and zero for the rest of the 3-month stress periods of a 5-year transient run of daily time steps for each of the pumping and injection wells in a flat-head simulation model. Responses at all wells are observed over the 20 seasonal stress periods. These response coefficients are then gathered together to form the response matrix. The repeated runs of the simulation model are executed 21 times for each of the water supply and containment wells in the single-layered cases and 57 times for each of the water supply and containment wells in the multi-layered cases.

The well configuration used for the creation of the response equations are shown in the following figures. Figure 4.1 shows the water supply and containment wells used for the one-layered constant- and variable-density cases, whereas Figures 4.2, 4.3 and 4.4 show the water supply and containment wells used in the five-layered cases. For the five-layered simulations, the water supply wells are assigned to the middle (3^{rd}) layer only and the containment wells are assigned to the top (1^{st}) layer, middle (3^{rd}) layer and the bottom (5^{th}) layer.

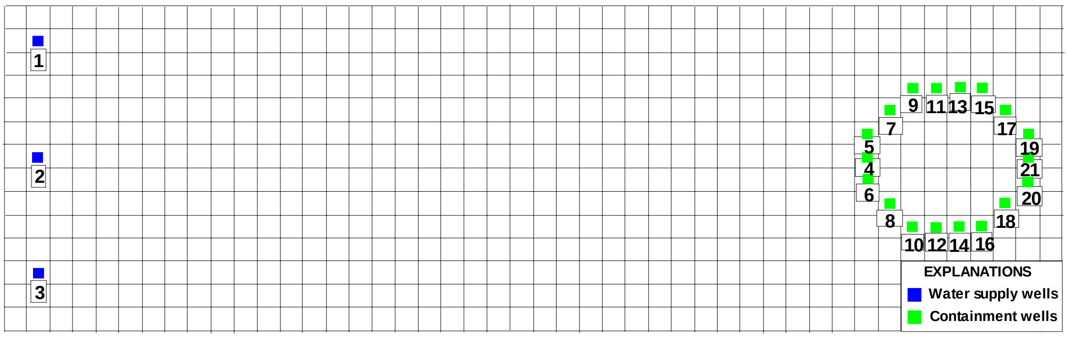


Fig. 4.1 Well configuration for the one-layered aquifer system.

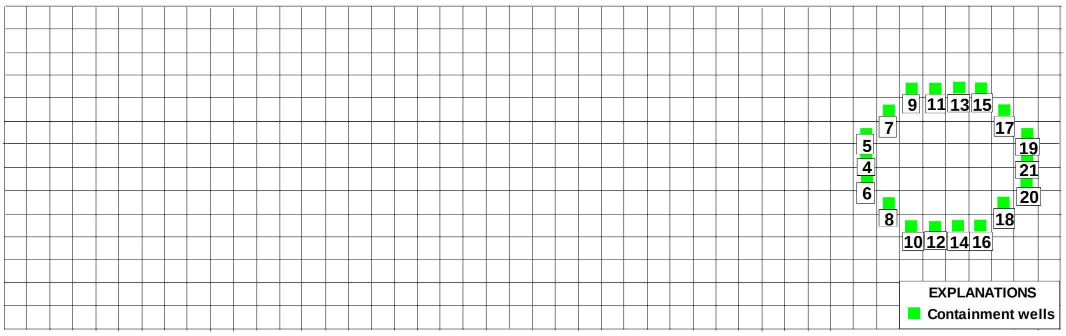


Fig. 4.2 Well configuration for the five-layered aquifer system showing the top (1st) layer only.

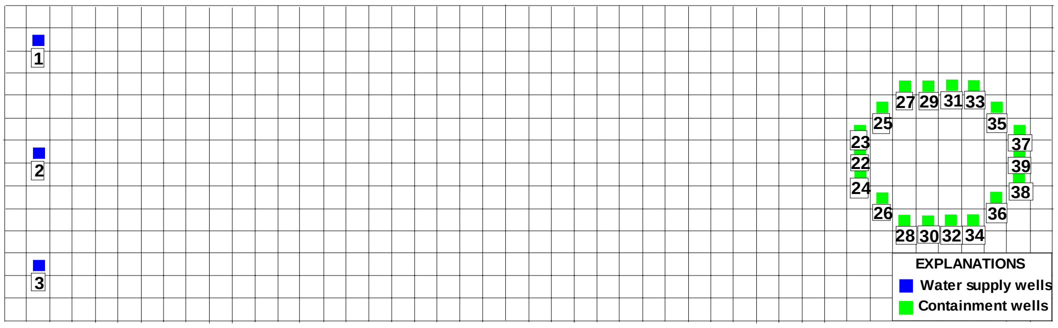


Fig. 4.3 Well configuration for the five-layered aquifer system showing the middle (3rd) layer only.

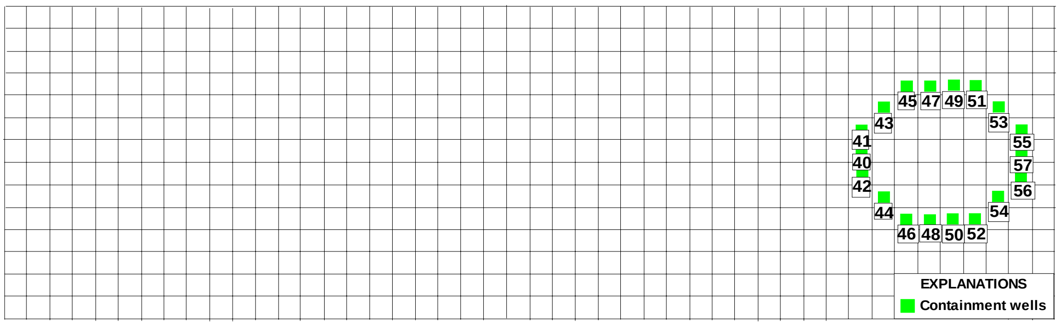


Fig. 4.4 Well configuration for the five-layered aquifer system showing the bottom (5th) layer only.

CHAPTER 5

OPTIMIZATION MODEL

A linear optimization model combined with groundwater flow and transport simulation is formulated to choose wells among a set of potential wells located at the perimeter of the freshwater mound and arrange their pumping/injection schedules so that the mound is kept from migrating subject to a series of system constraints. The objective (5.1) is to minimize the sum of pumping and injection rates of hydraulic gradient control wells while maintaining zero gradients at the freshwater mound boundaries:

$$Min Z = \sum_{k=4}^{M} \sum_{n=1}^{N} Q(k,n) \tag{5.1}$$

where *Z* is the sum of pumping and injection rates ($m^3\ s^{-1}$), *Q(k,n)* is the average discharge/injection rate at pumping/injection well *k* during pumping period *n* ($L^3\ T^{-1}$), *M* is the total number of injection and pumping wells, and *N* is the total number of time periods that comprise the whole planning horizon consisting of 20 three-month periods.

The locations of the hydraulic gradient control pairs and the potential containment wells are shown in Figures 5.1, 5.2, 5.3 and 5.4 for the single- and multi-layered cases, respectively. The gradient control wells are located in such a way that each of them makes a couple with the one just below or next to it depending on the target gradient directions. The gradient control pairs are successively numbered so that the well with the greater number in a pair always indicates the proposed inward gradient toward the freshwater mound.

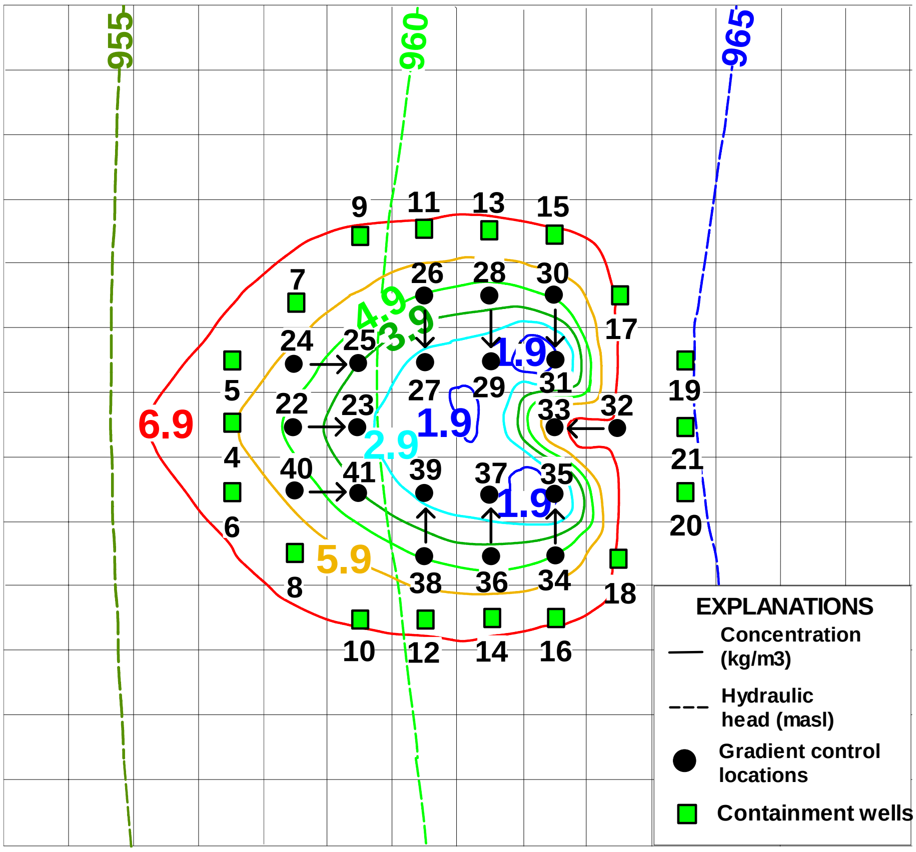


Fig. 5.1 Locations of gradient control pairs and potential containment wells for the single-layered constant- and variable-density cases.

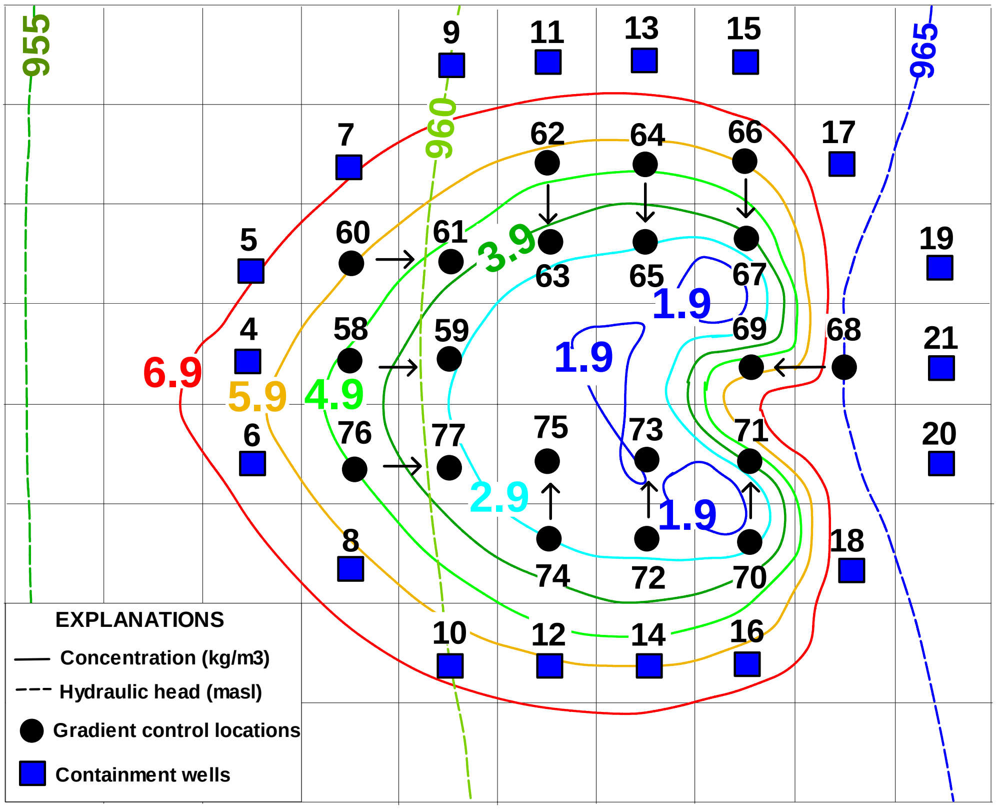


Fig. 5.2 Locations of gradient control pairs and potential containment wells for the multi-layered constant- and variable-density cases showing the top layer.

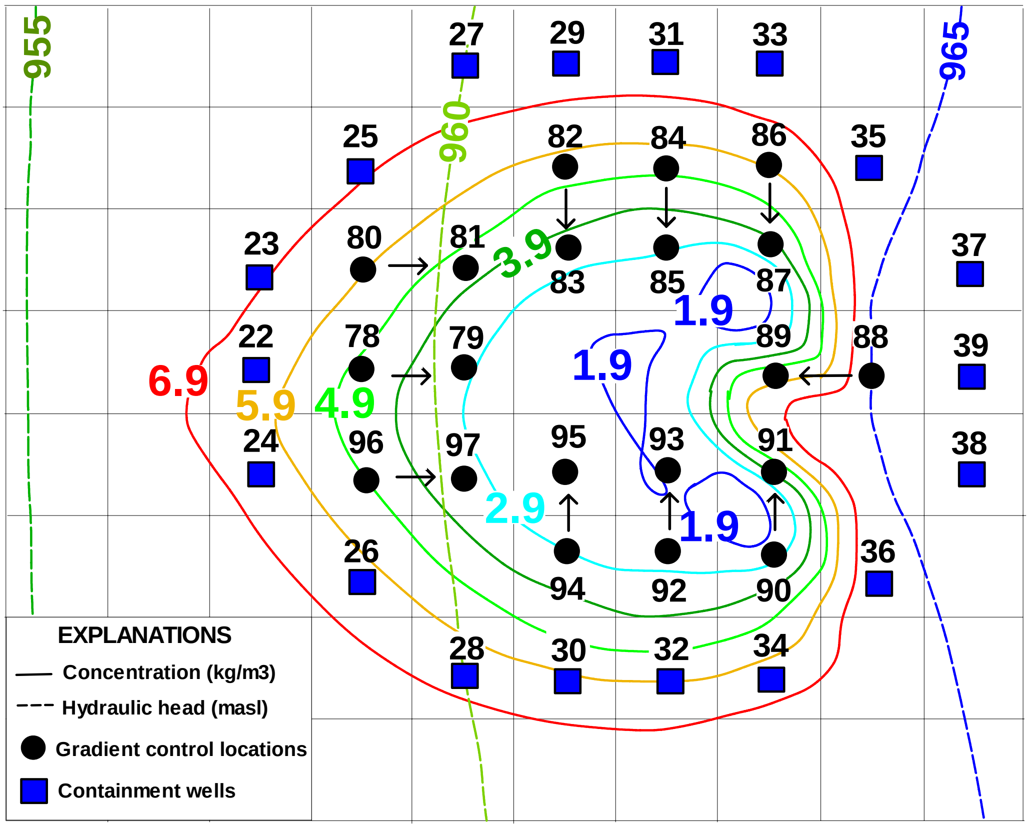


Fig. 5.3 Locations of gradient control pairs and potential containment wells for the multi-layered constant- and variable-density cases showing the middle layer.

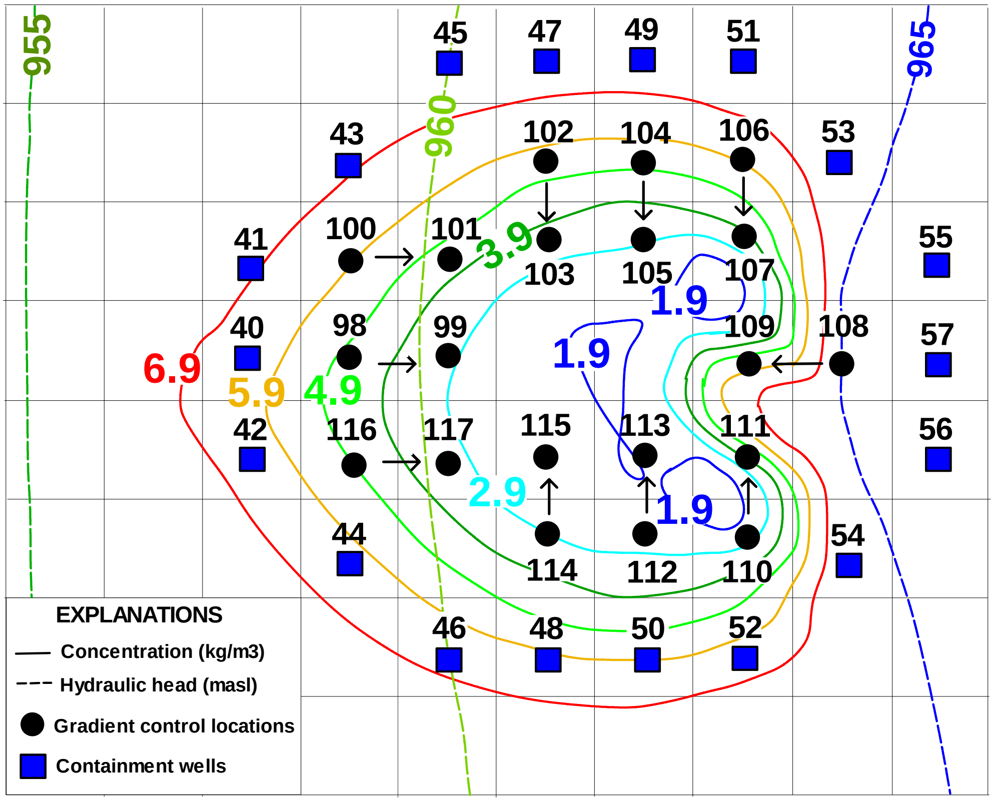


Fig. 5.4 Locations of gradient control pairs and potential containment wells for the multi-layered cases showing the bottom layer.

The optimization model is subject to a set of constraints including the systems response equations, demand requirements, hydraulic gradient controls, pumping and injection limitations which are explained below:

1. Water demand constraints

   Water demand from 3 existing water supply wells during each planning period, *D(n)*, must be satisfied:

$$\sum_{k=1}^{3} Q(k,n) \geq D(n) \qquad \forall n \qquad (5.2)$$

2. Response equations

The continuity of the system must be maintained by satisfying the response equations:

$$d(k,n) = \sum_{j=1}^{M}\sum_{i=1}^{n} \beta(k, j, n-i+1)Q(j,i) \qquad \forall n, \forall k \quad (5.3)$$

$$s(k,n) - u(k,n) = \sum_{j=1}^{M}\sum_{i=1}^{n} \beta(k, j, n-i+1)Q(j,i) \qquad \forall n, \forall k \quad (5.4)$$

where *d(k,n)* represents the drawdown/build-up at pumping/injection well *k* at the end of planning period *n* (L), which is replaced by the difference of two non-negative variables, *s(k,n) and u(k,n),* in order to remove the unrestricted variable and allow the linear program to choose either pumping or recharge for each well. The *s(k,n)* = drawdown at pumping well *k* at the end of planning period *n* (L), *u(k,n)* = build-up at injection well *k* at the end of planning period *n* (L), *β(k, j, n – i + 1)* = drawdown/build-up response function at the *k*th well at the end of *n*th period due to a unit pumping/injection at the *j*th well applied throughout the *i*th period (T L^{-2}).

3. Hydraulic gradient constraints

Gradient at control pairs have to be maintained to direct the gradient inward toward the freshwater mound:

$$[s_{in}(k,n) - u_{in}(k,n)] - [s_{out}(k,n) - u_{out}(k,n)] \geq H_{in} - H_{out} \quad \forall n_{pair}, \forall n \ (5.5)$$

where H_{in} is the hydraulic head at a point outside the mound and H_{out} is the hydraulic head at a point inside the mound where the responses at each pair of the nodes on either side of the mound boundary are converted into a gradient response (Gorelick and Atwood, 1984).

4. Total injection rate must not exceed total pumping rate

$$\sum_{k=1}^{3} Q(k,n) + \sum_{k \in NP} Q(k,n) - \sum_{k \in NI} Q(k,n) \geq 0 \qquad \forall n \tag{5.6}$$

where *NP* = set of pumping wells, *NI* = set of injection wells.

5. Pumpage/injection upper and lower bounds

Pumpage/injection rate at each pumping/injection well must not exceed the specified upper bounds, $Q_{max}(k)$.

$$Q(k,n) \leq Q_{\max}(k) \qquad \forall n, \forall k \tag{5.7}$$

The lower bounds with the exception of water supply wells are set to zero. At supply wells, the lower bound at each well is specified to be 1/3 of the D(n).

The computer programs are coded in a Fortran-90 compiler and executed to generate the coefficient matrices of the model in the standard MPS format. The resulting matrix for the single-layer cases contains 2420 decision variables (columns) and 1062 constraints (rows) whereas it contains 6900 decision variables (columns) and 2982 constraints (rows) for the five-layered cases. The linear optimization model is solved by using the CPLEX (*Cplex Optimization Inc.*, 1995) algorithm, which is a tool for solving linear, mixed-integer or quadratic programming type problems. The optimization models for the one- and five-layered cases are listed in Appendices A and B.

CHAPTER 6

NUMERICAL APPLICATION OF THE MANAGEMENT MODELS

The proposed management models are applied to the hypothetical groundwater system in order to achieve the optimal capture and containment of the freshwater mound while satisfying the limitations and requirements explained in detail in Chapter 5. A total management period of five years is considered to be sufficient for the complete containment of the mound.

The upper bounds of pumpage and injection at water supply and containment wells at each period are set to 60 L s^{-1} which is assumed to be the maximum value for the capacity of a well. The lower bounds at all wells are set to zero except the water supply wells. At the water supply wells, the lower bound at each well is specified to be the 1/3 of the demand value that is equal to 15 L s^{-1} for each time period.

The total demand for the whole management period is calculated by assuming seasonal demand, meaning that water requirements increase in summer months and decrease in the winter. According to this assumption, the average water demand values for the first, second, third, fourth and fifth years are 50 L s^{-1}, 55 L s^{-1}, 60 L s^{-1}, 65 L s^{-1}, and 70 L s^{-1} respectively. Figure 6.1 shows the increasing demand according to seasons for a five-year planning period.

The maximum allowable drawdown at all supply and injection wells are defined as 100 m for all pumping periods.

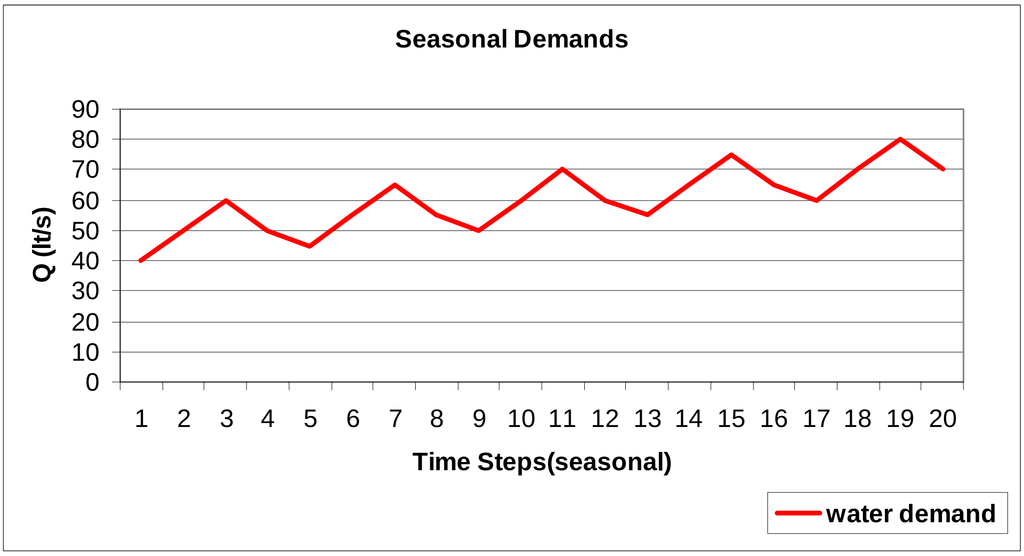


Fig. 6.1 A chart showing the seasonal demands for a 5-year planning period.

The effects of fluid density on groundwater flow and solute transport are further considered in details by solving the hypothetical model as a constant-density and a variable-density problem. The model has been simulated first by assuming constant-density flow and then re-simulated by activating the variable-density flow process. The linear optimization model combined with the groundwater management model is solved one by one for single- and multi-layered aquifer systems characterized by constant-density flow and variable-density flow using the CPLEX algorithm. The necessary data files for the optimization models (the MPS files) are generated by using the programs written in FORTRAN-90 computer code which are listed in Appendices A and B. Evaluations of the optimal pumping policies are made by simulating the SEAWAT-2000 groundwater flow and transport model.

The solutions of the models yield the seasonal (3-month) optimal rates at each pumping and injection wells while achieving the optimal containment under the objective of minimizing discharge and recharge rates.

Case 1 Constant-density flow in a single-layered aquifer:

Applying the parameters stated above the coupled simulation-optimization type groundwater management model is solved for constant-density flow in a single-layered aquifer and an objective value of 2.71 $m^3 s^{-1}$ is obtained. The optimal solution of the model has selected to use the 18^{th} and 20^{th} wells which are located on the up-gradient of the mound for pumpage whilst the wells numbered as 4, 5, 6, 11, and 12 that are located on the down-gradient are utilized as injection wells (Fig. 6.2).

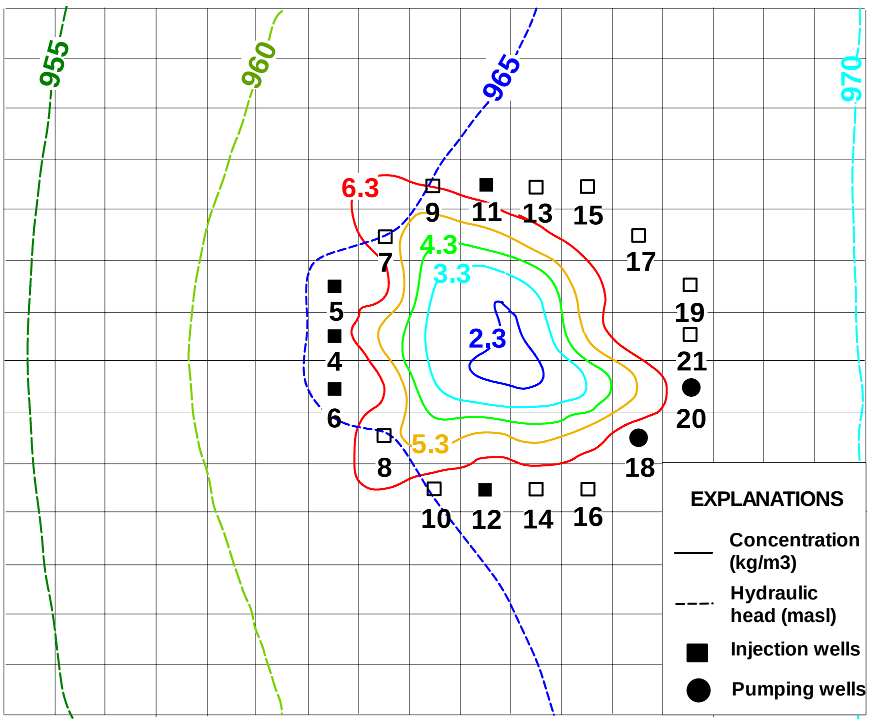


Fig. 6.2 Close-up view of the contained mound, injection and pumping wells for Case1 at the end of the planning period.

The optimal pumpage and injection rates are input back to the transient flow and transport model to check if the constraints are satisfied. The outcomes clearly indicate that the freshwater stored is kept from migration through the use of optimal hydraulic gradient control wells which create a zero gradient around the freshwater mound boundary. The concentration and the hydraulic head distributions of the mound after the optimal schedules applied are presented in Figure 6.2.

Different pumpage and injection rates associated with each well are shown in Figure 6.3. It is clear from the figure that the 5^{th} and 6^{th} wells are operated as the main injection wells whereas the 20^{th} well is operated as the main pumping well. The well no.11 may be disregarded due to its very low injection rate. The total pumpage rate from the pumping wells is 1.36 $m^3 s^{-1}$, exactly the same as the total injection rate that sum up to 2.72 $m^3 s^{-1}$ in overall. The amount of water reserved for the demand is supplied from the water supply wells and equals 1.20 $m^3 s^{-1}$. This amount is not integrated into the objective value.

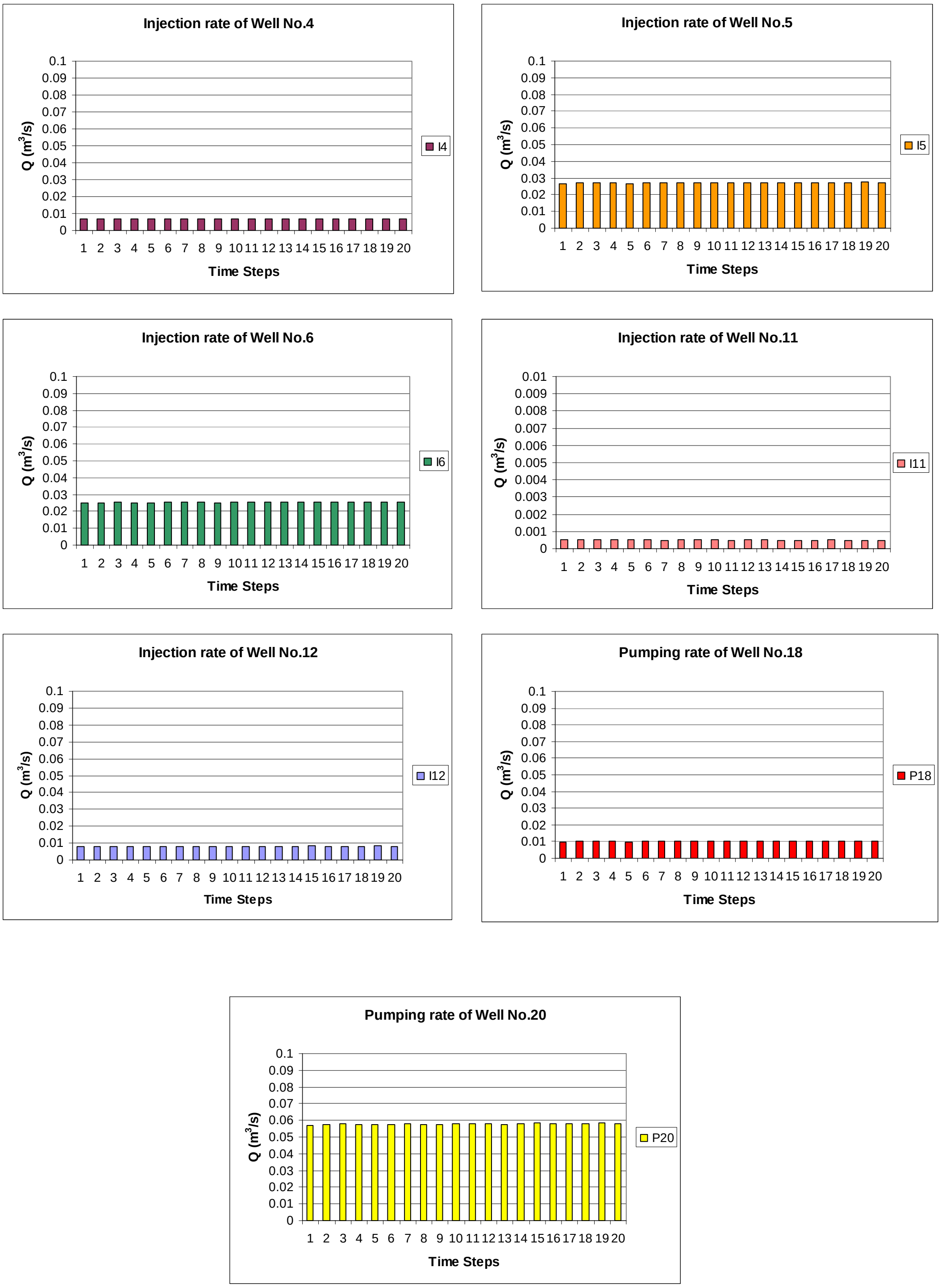


Fig. 6.3 Optimal injection and pumping schedules obtained from the optimization model for Case1.

When the model is solved once more without imposing any upper bounds on pumping and injection wells, the objective value and the pumping/injection rates remain the same (Figures 6.4 and 6.5).

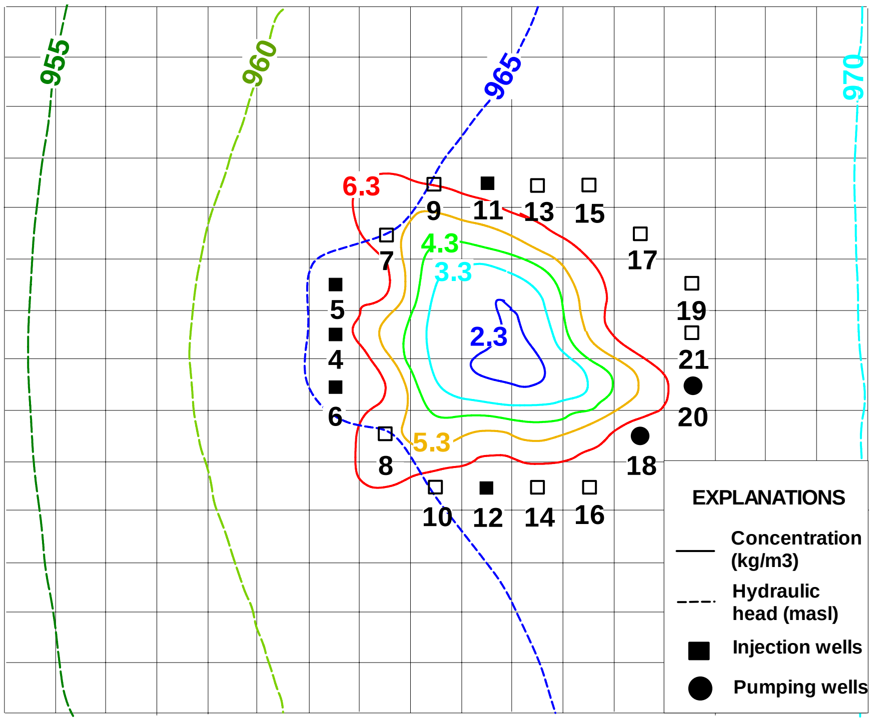


Fig. 6.4 Close-up view of the contained mound, injection and pumping wells for Case1 at the end of the planning period without upper bounds.

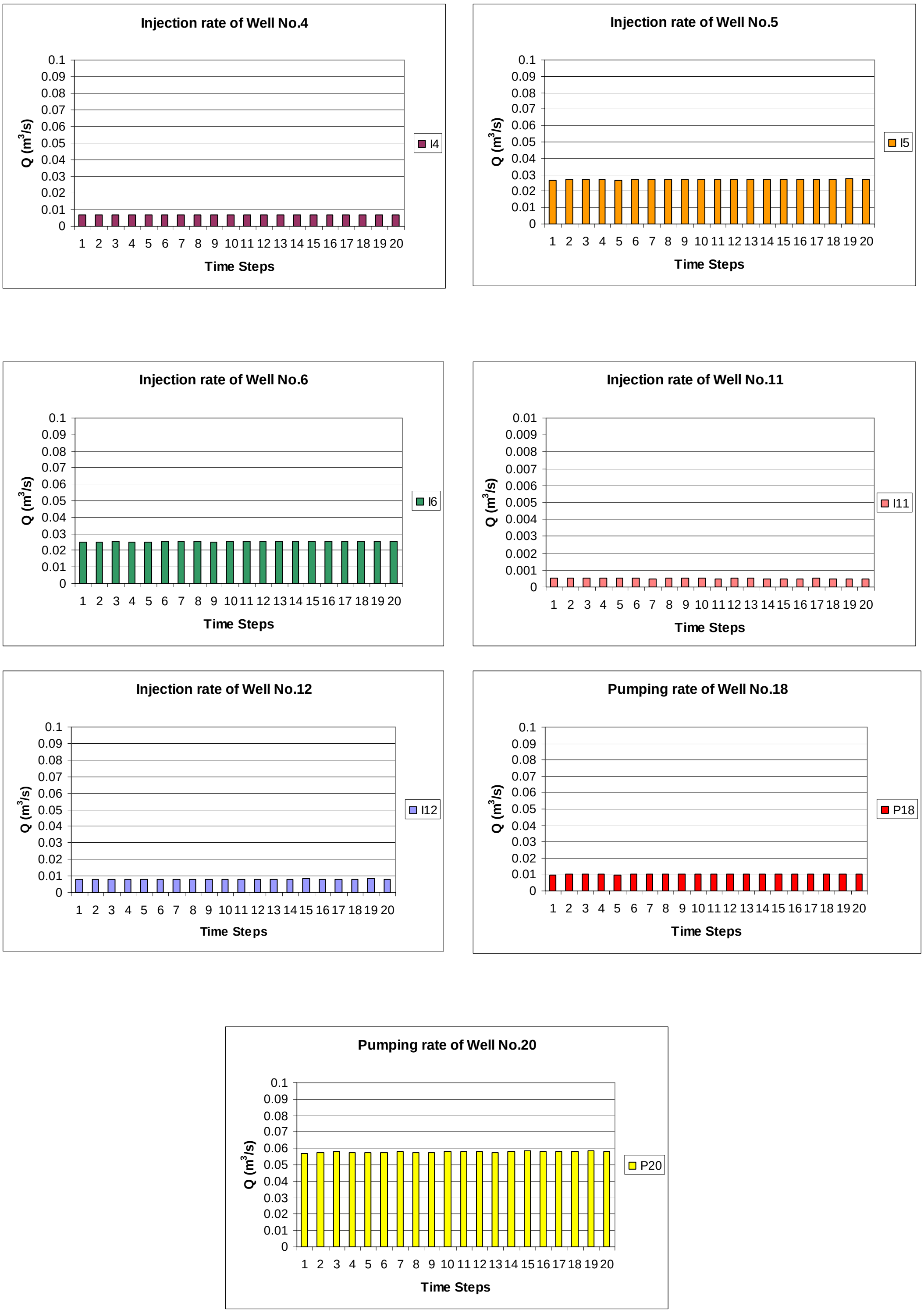


Fig. 6.5 Optimal injection and pumping schedules obtained from the optimization model for Case1 without upper bounds.

Figure 6.6 shows the pumping and injection rates according to the time steps for Case 1. As it can be seen from the figure, the demand is increasing seasonally. The pumping and injection rates show very little inclination during the whole planning period and are equal to each other.

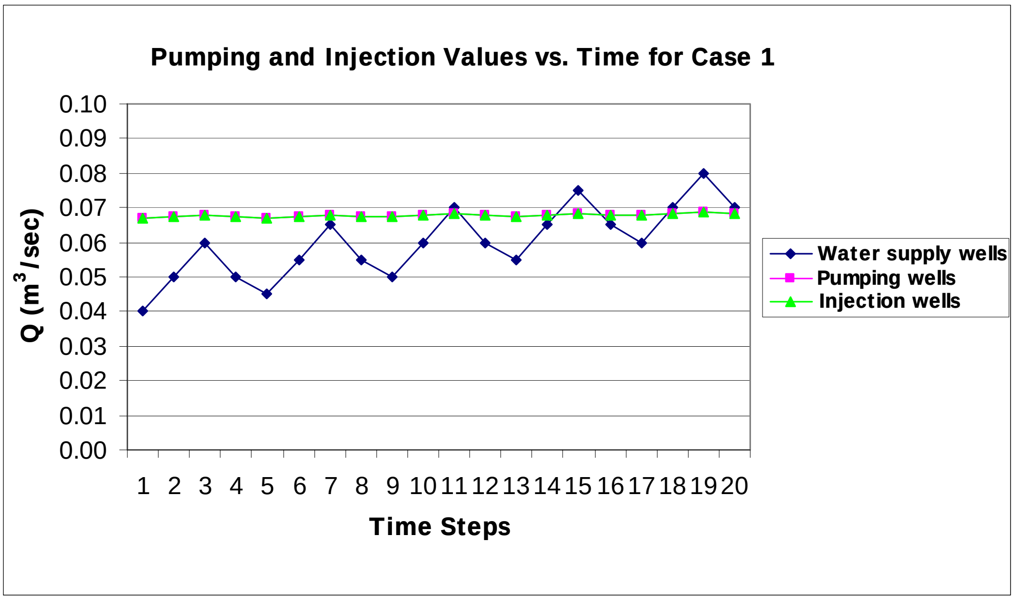


Fig. 6.6 Pumping and injection rates versus time for Case1 during the whole planning period.

Case 2 Constant-density flow in a multi-layered aquifer:

In this case, the coupled simulation-optimization type groundwater management model is solved for constant-density flow in a five-layered aquifer system with upper bounds on pumping and injection wells as 60 L s^{-1}. The objective function value of 2.71 m^3 s^{-1} is exactly equal to the value obtained in Case 1. The optimal solution of the model has operated the 20th well in the top layer (Fig. 6.7), the 36th and 38th wells in the third layer (Fig. 6.8), and the 56th well at the bottom layer (Fig. 6.9) for pumpage. All of them are located on the up-gradient of the mound. On the other hand, the down-gradient wells numbered as 5, 6, 11, 12 at the top layer (Fig. 6.7), 22, 24, 29, 30 at the third layer (Fig. 6.8) and 41, 42, 47 and 48 at the bottom layer (Fig. 6.9) are selected as injection wells.

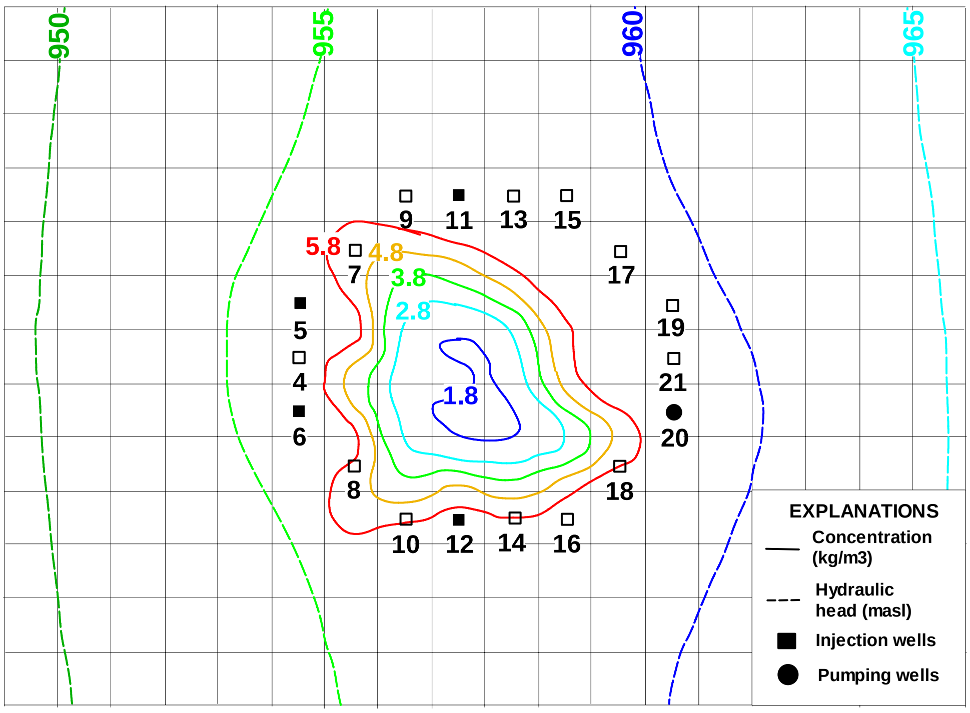


Fig. 6.7 Close-up view showing the top layer of the contained mound, injection and pumping wells for Case2 at the end of the planning period.

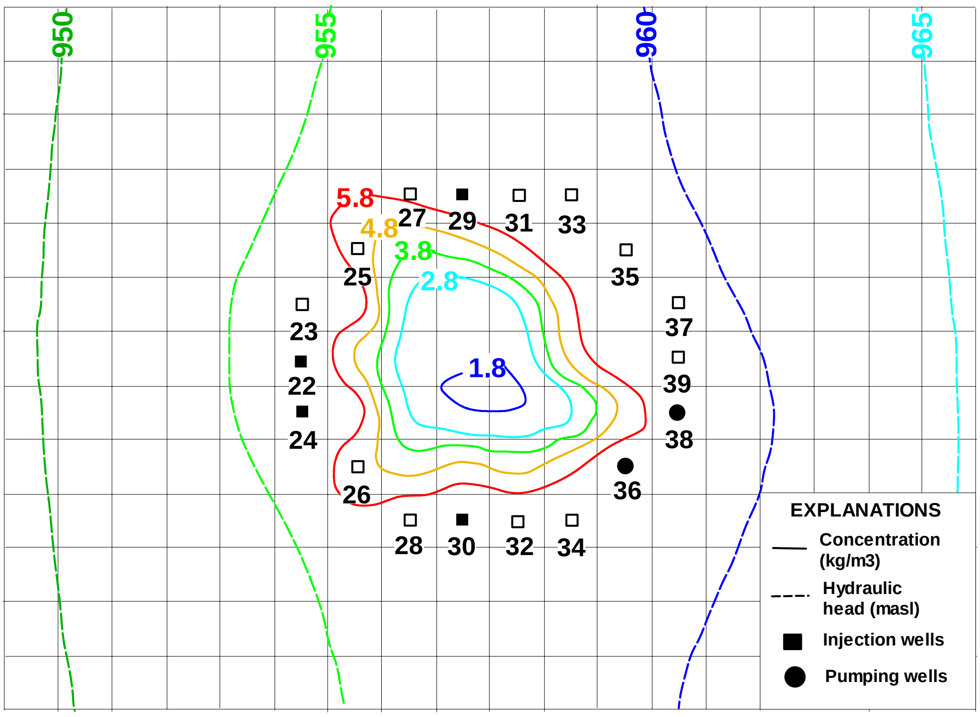


Fig. 6.8 Close-up view of the middle layer of the contained mound, injection and pumping wells for Case2 at the end of the planning period.

The optimal pumpage and injection rates are input back to the transient flow and transport model to check if the constraints are satisfied. The results show that the freshwater mound is successfully held in its original location through the use optimal hydraulic gradient control wells by creating a flat gradient around the freshwater mound boundary. The concentration and the hydraulic head distributions at the end of the planning period after the optimal schedules applied are presented in Figures 6.7, 6.8 and 6.9. As it can be seen from the figures, the hydraulic head and the concentration values remain constant in the vertical direction throughout all the layers. Figures 6.10 and 6.11 show the vertical distributions of concentration and head values along a cross-section taken at y = 5100 m, respectively.

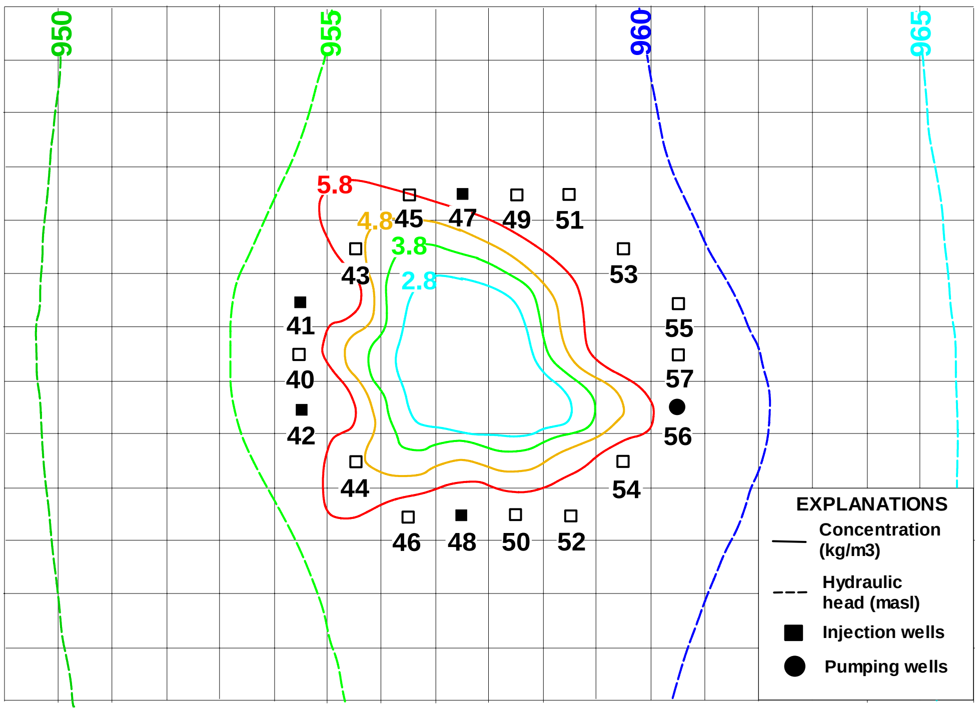


Fig. 6.9 Close-up view of the bottom layer of the contained mound, injection and pumping wells for the Case2 at the end of the planning period.

Different pumpage and injection rates associated with each well are shown in Figure 6.12. When the figure is observed, it is seen that the main pumping wells are the 20th and 56th wells. The 38th well may be shut down since it operates only once during the whole planning period. Among the injection wells, the 11th, 29th, 47th, and the 48th wells operate less than the others. The 30th well can be closed since it operates only three times during the whole planning period. The total pumpage from the pumping wells is 1.357 $m^3\ s^{-1}$ which is equal to the total injection amount summing up to 2.71 $m^3\ s^{-1}$in overall. The amount of water reserved for the demand is supplied from the water supply wells and equals 1.20 $m^3\ s^{-1}$ as in the previous case. This amount is not included in the objective value.

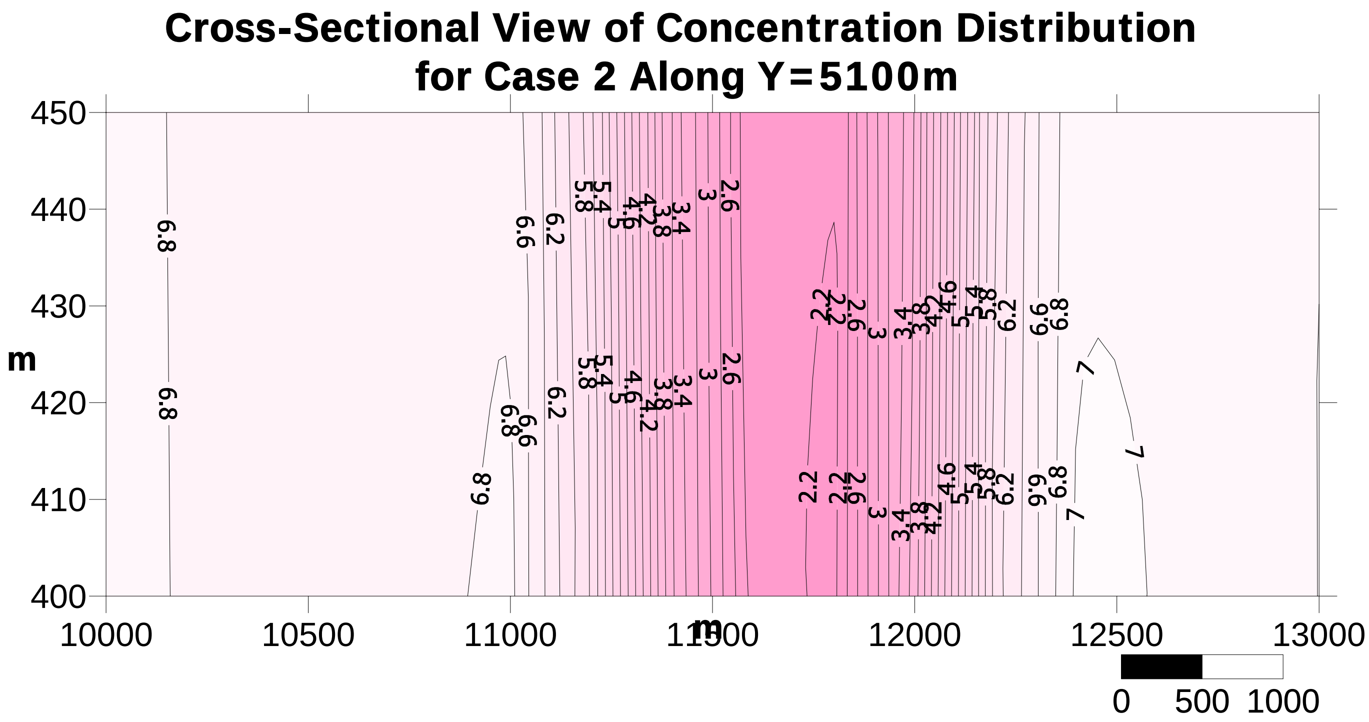


Fig. 6.10. Cross-sectional view of concentration distribution for Case 2 along y = 5100 m at the end of the planning period.

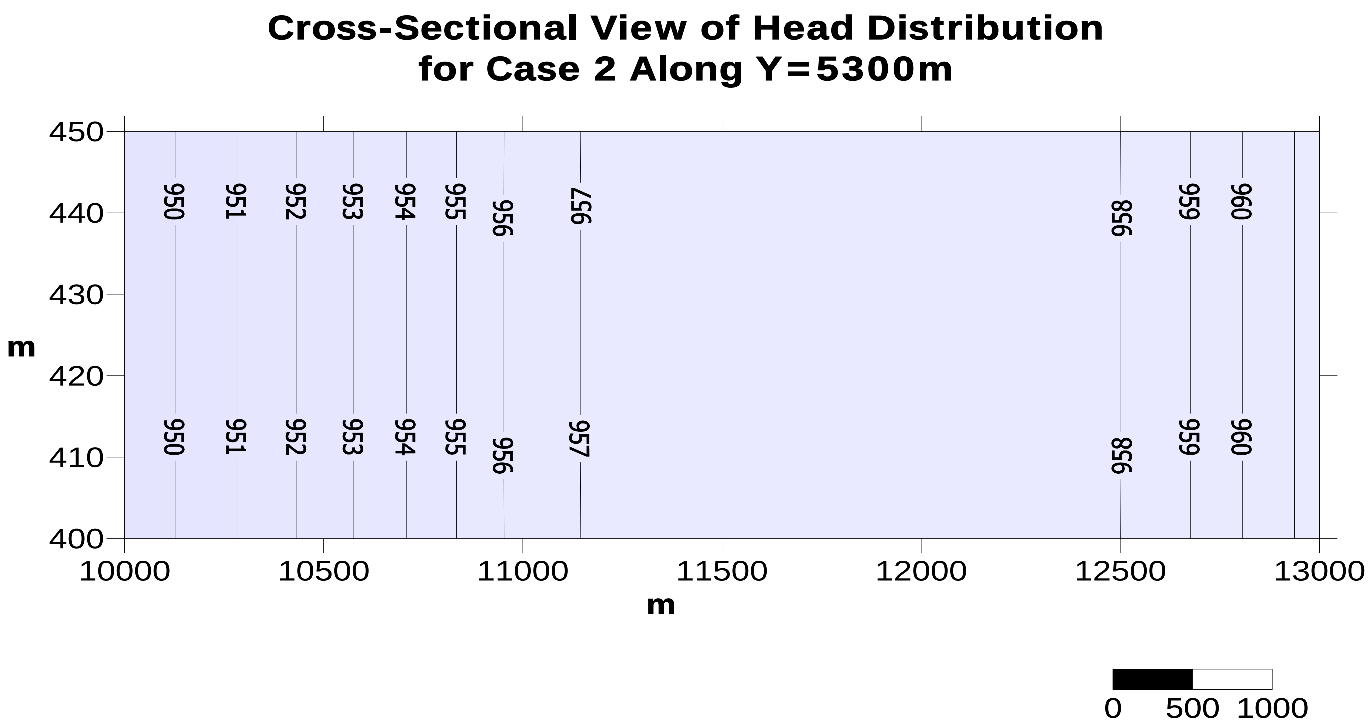


Fig. 6.11 Cross-sectional view of head distribution for Case 2 along y = 5100 m at the end of the planning period.

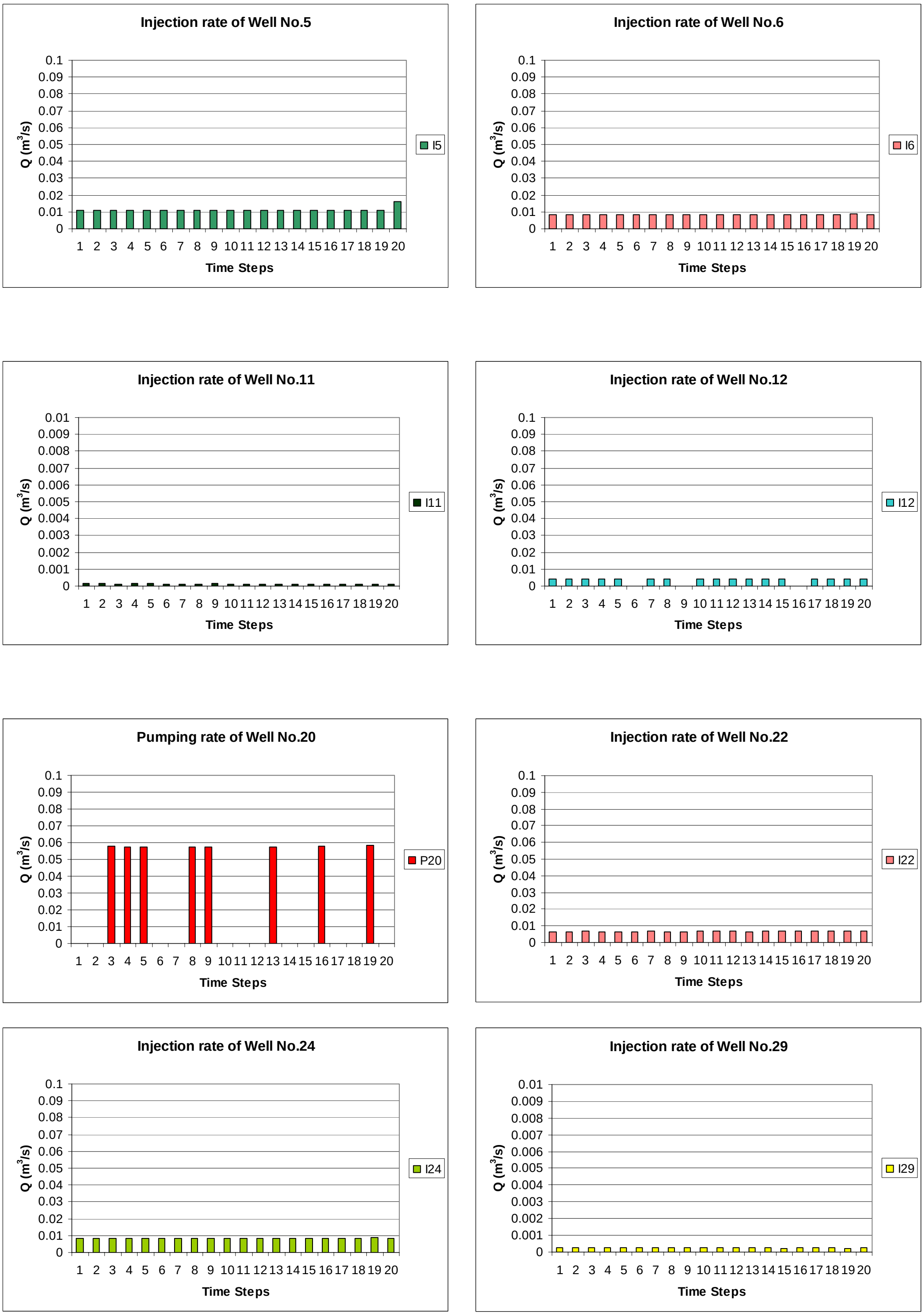


Fig. 6.12 Optimal injection and pumping schedules obtained from the optimization model Case2.

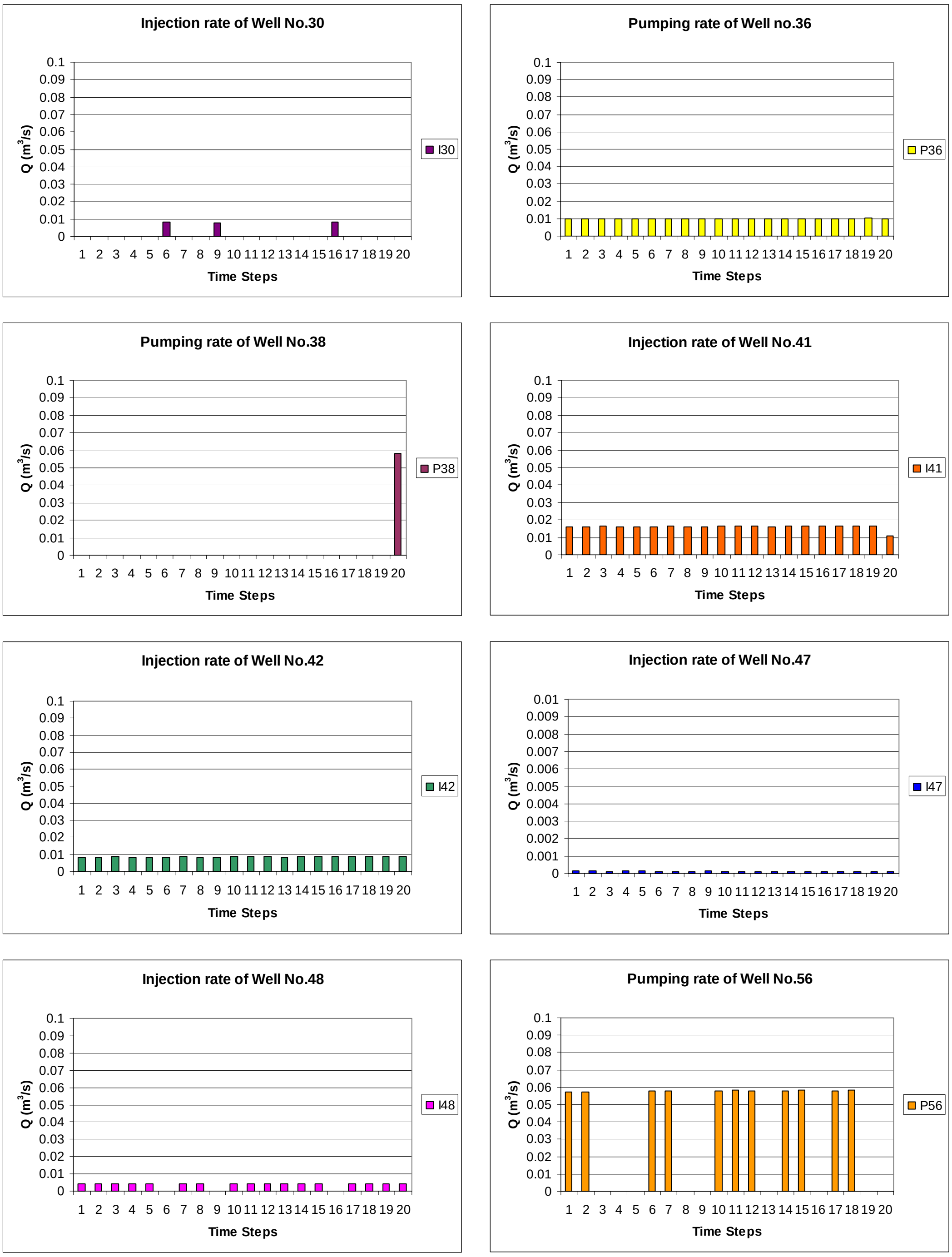


Fig. 6.12 (Continued)

Figure 6.13 shows the pumping and injection rates according to the time steps for Case 2. According to the figure, the pumping and injection rates show very little inclination during the whole planning period and are equal to each other. The demand increases seasonally.

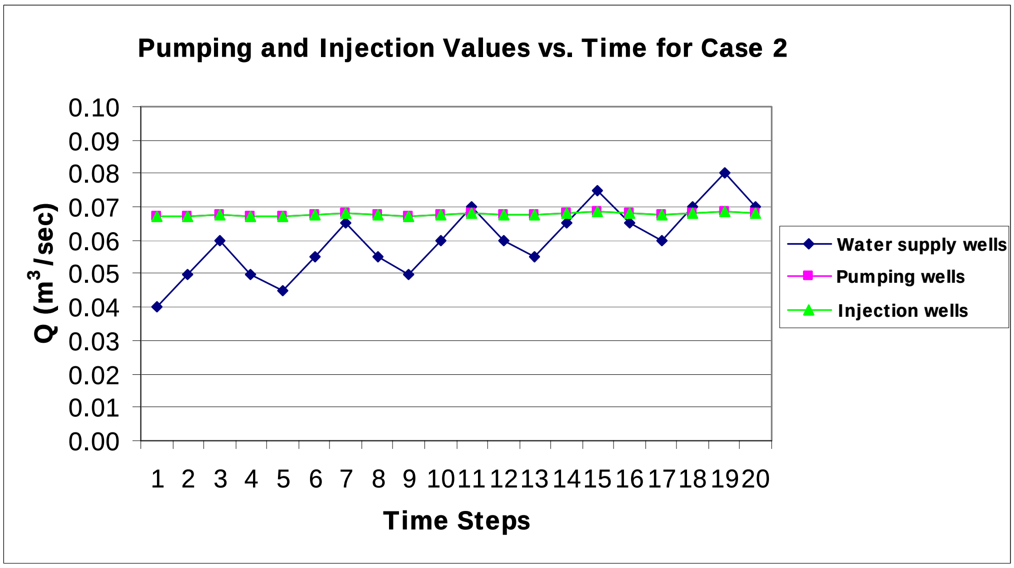


Fig 6.13 Pumping and injection rates versus time for Case2 during the whole planning period.

Case 3 Variable-density flow in a single-layered aquifer:

Application of the optimization model to the hypothetical groundwater system for variable-density flow in a single-layered aquifer resulted as being infeasible when the upper bounds of pumping and injection on wells are set to 60 L s^{-1}. In order to remove the infeasibility, the upper bounds are increased to 70 L s^{-1}, 80 L s^{-1} and 90 L s^{-1}. However, the model still remains infeasible until the upper bounds are totally removed. An objective value of 17.64 m^3 s^{-1} is obtained without any upper bounds of pumpage and injection specified on pumping and injection wells. The optimal solution selects the wells 17, 18, 19 and 20 located on the up-gradient of the mound as pumping wells while wells numbered as 5, 6, 11, 12, 13, 14 and 21 that are located on the down-gradient of the mound are used as injection wells (Fig. 6.14).

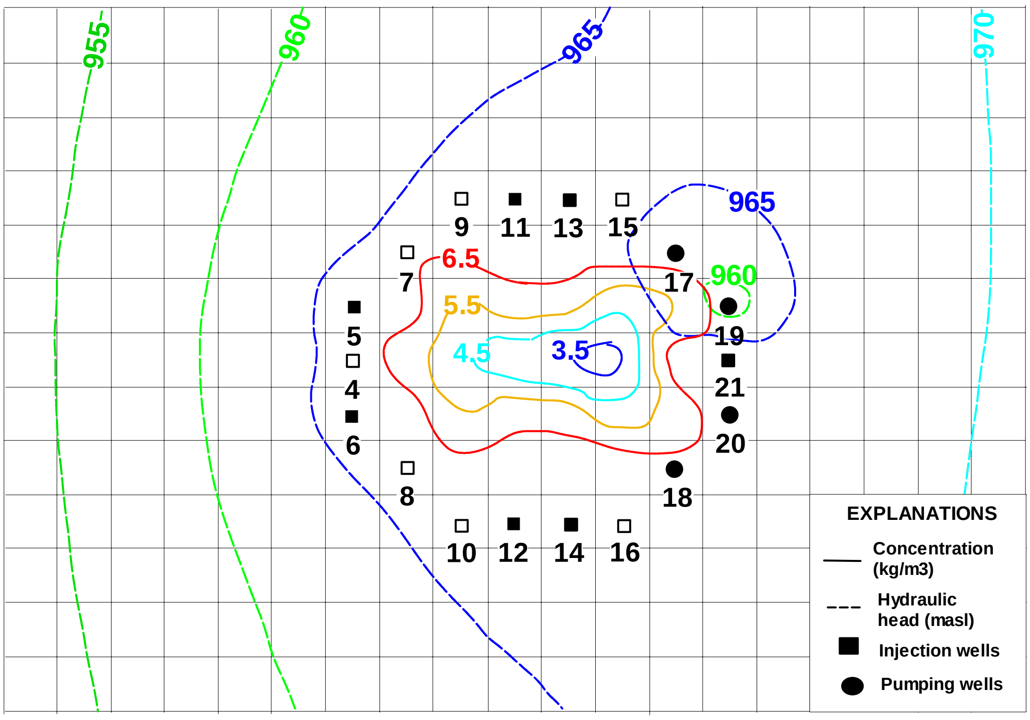


Fig. 6.14 Close-up view of the contained mound, injection and pumping wells for Case3 at the end of the planning period.

The optimal pumpage and injection rates are input back to the transient flow and transport model to check if the constraints are satisfied. The results of the model show that the freshwater mound is kept from migration by using optimal hydraulic gradient control wells that create a flat gradient around the freshwater mound boundary. The concentration and the hydraulic head distributions of the mound after the optimal schedules applied are presented in Figure 6.14.

Different pumpage and injection rates associated with each well are shown in Figure 6.15. The figure shows that the 13^{th} and 14^{th} wells inject so little water that they may be left deactivated. On the other hand, the 17^{th} and the 18^{th} wells pump less water than the 19^{th} and 20^{th} wells pump. The total pumpage from the pumping wells is 8.71 m^3 s^{-1} whereas the total injection rate is equal to the 8.93 m^3 s^{-1} making a total of 17.64 m^3 s^{-1}. The amount of water reserved for the demand is supplied from the water supply wells and equals 1.60 m^3 s^{-1}. This amount is considered separately from the objective value. The sum of total pumpage and the demand value together makes a bigger amount than that of the injection which proves that the fourth constraint explained in Chapter 5 is satisfied.

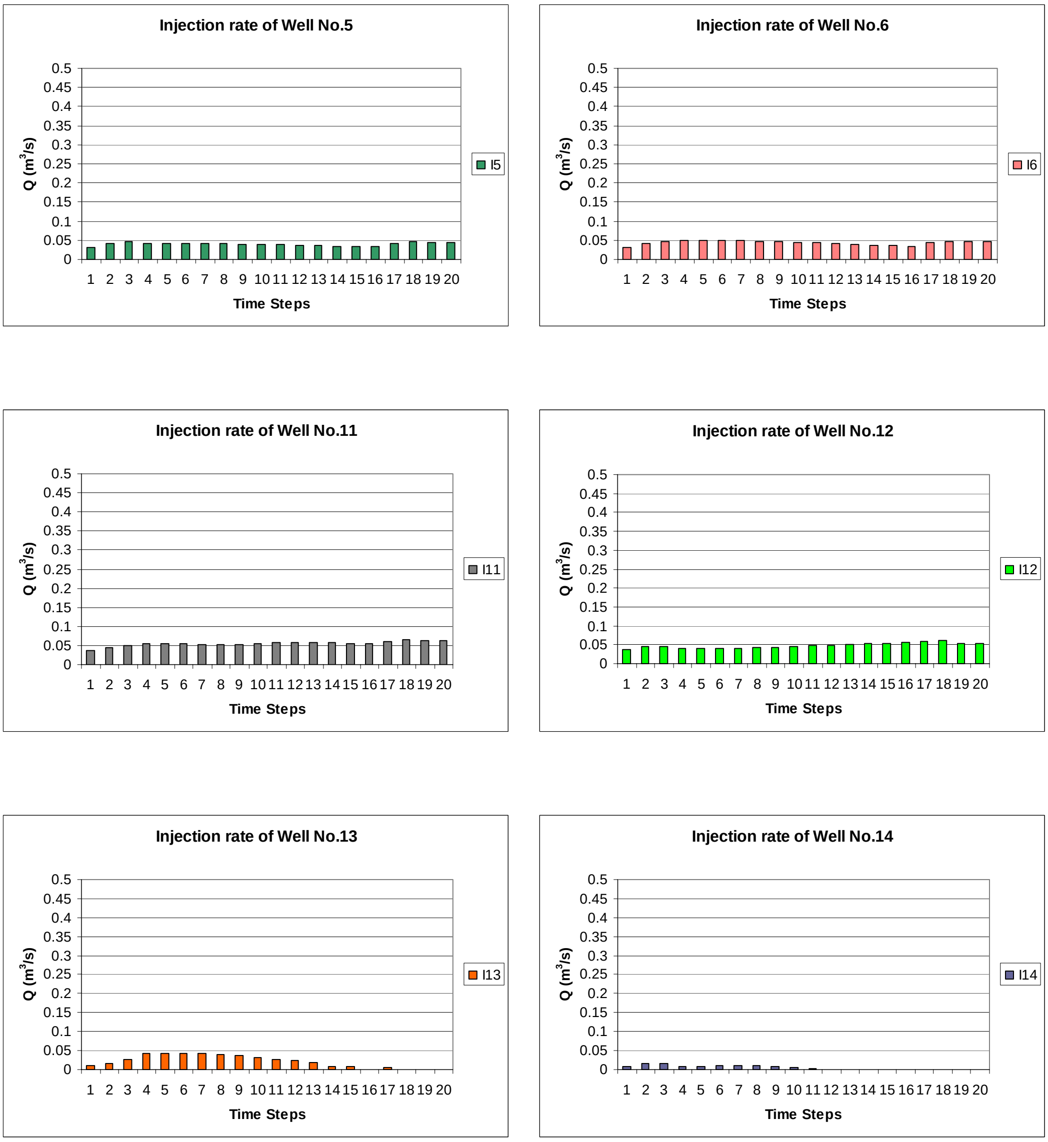


Fig. 6.15 Optimal injection and pumping schedules obtained from the optimization model for Case3.

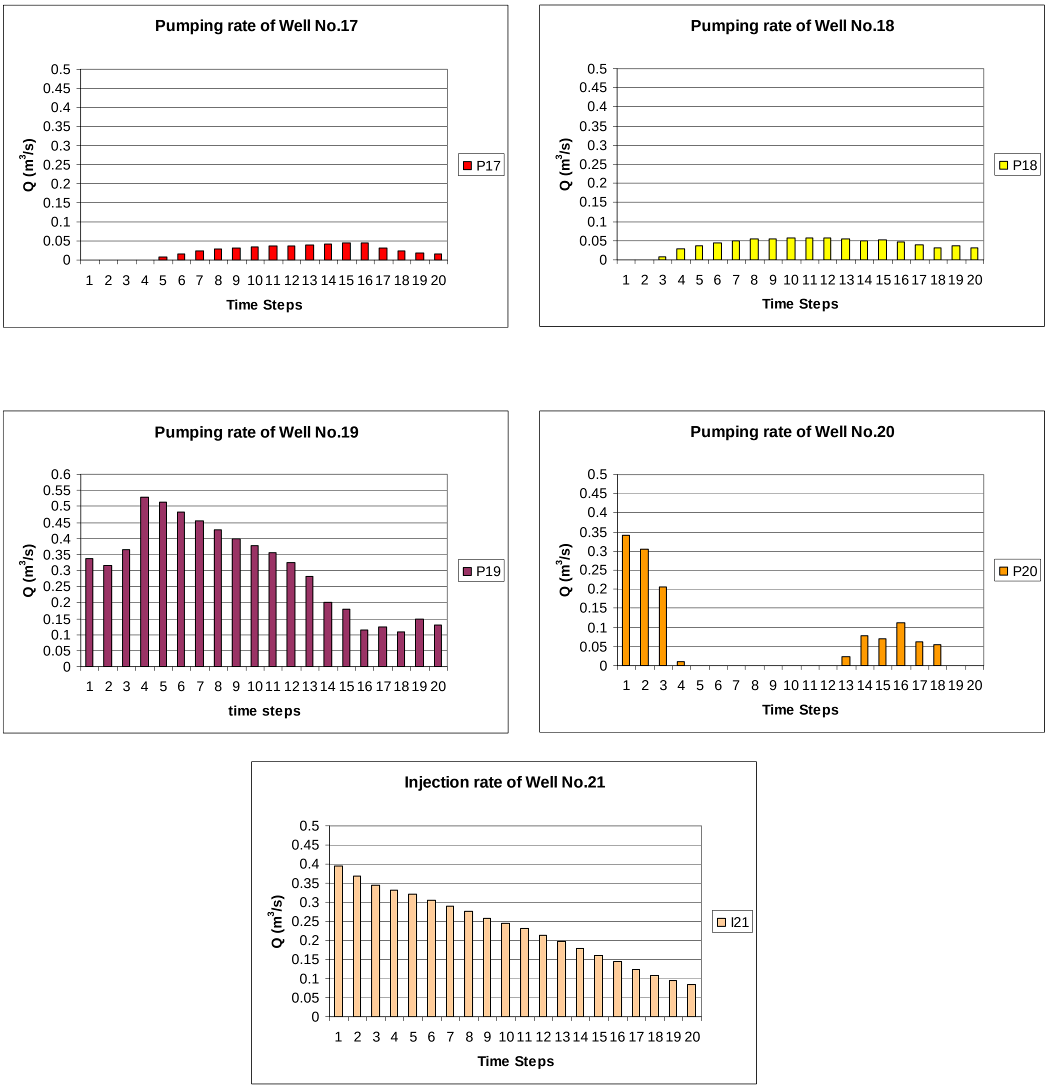


Fig. 6.15 (Continued)

Figure 6.16 shows the pumping and injection rates according to the time steps for Case 3. The demand increases seasonally as in the constant-density cases for one- and multi-layer systems but the pumping and injection rates show significant declination during the whole planning period in contrary to the constant-density cases.

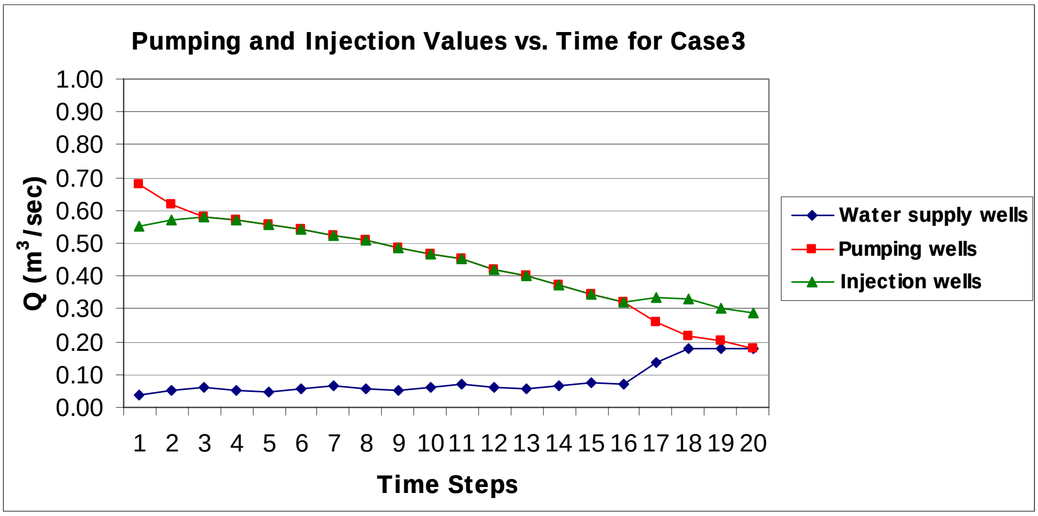


Fig. 6.16 Pumping and injection rates versus time for Case3 during the whole planning period.

Case 4 Variable density flow in a multi-layered aquifer:

Application of the optimization model to the hypothetical groundwater system for variable-density flow in a five-layered aquifer has provided an optimal objective value of 17.42 L s^{-1} when the upper bounds of pumping and injection on pumping and injection wells are set to 60 L s^{-1}. If the upper bounds are increased to 70 L s^{-1}, 80 L s^{-1} and 90 L s^{-1}, the optimal objective values change as 17.28 L s^{-1}, 17.22 L s^{-1} and 17.19 L s^{-1} respectively. However, when no upper bounds of pumpage and injection are imposed on pumping and injection wells, an objective value of 17.07 m^3 s^{-1} is obtained which is accepted as the optimal solution for this case.

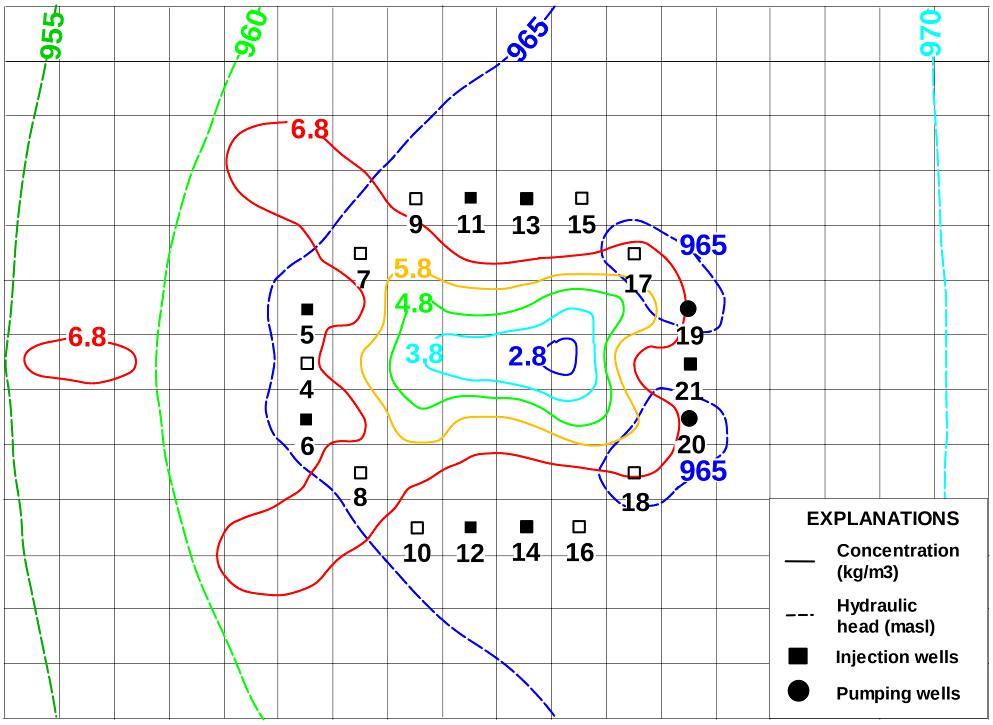


Fig. 6.17 Close-up view showing the first layer of the contained mound, injection and pumping wells for Case4 at the end of the planning period.

The wells 19 and 20 at the first layer (Fig. 6.17), well 37 at the third layer (Fig. 6.18), and 53, 54, 55 and 56 at the fifth layer (Fig. 6.19) that are located on the up-gradient of the mound are operated as pumping wells by the optimal solution. The wells 5, 6, 11, 12, 13, 14, 21, at the top layer, wells 23, 24, 29, 30, 31, 32, 39 at the middle layer, and wells 41, 42, 47, 48, 49 and 57 at the bottom layer are operated as injection wells.

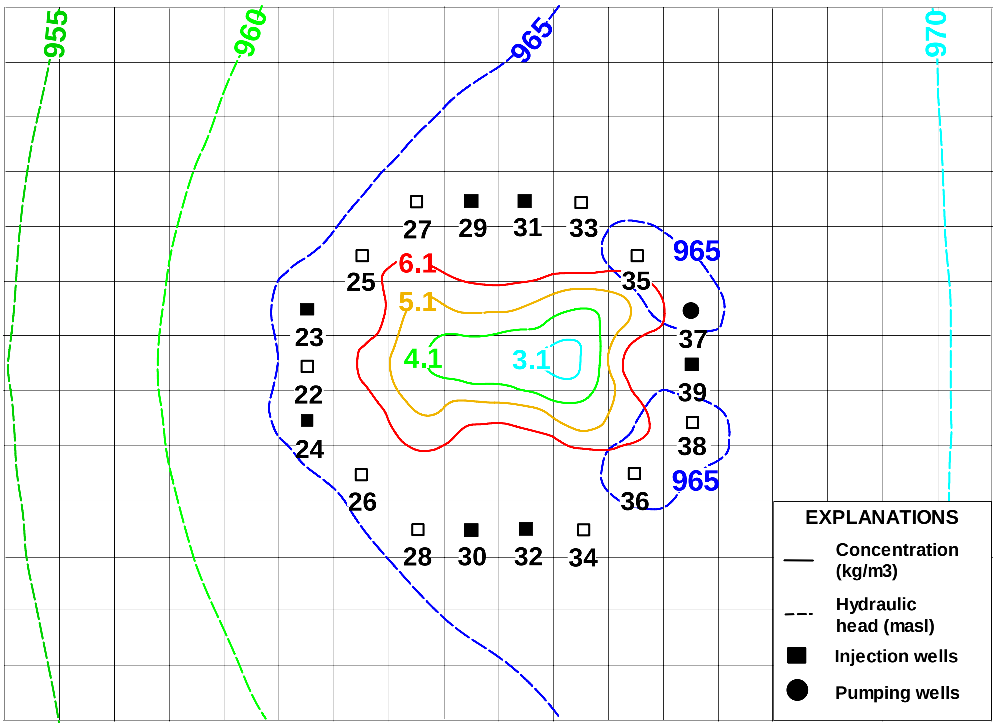


Fig. 6.18 Close-up view showing the third layer of the contained mound, injection and pumping wells for Case4 at the end of the planning period.

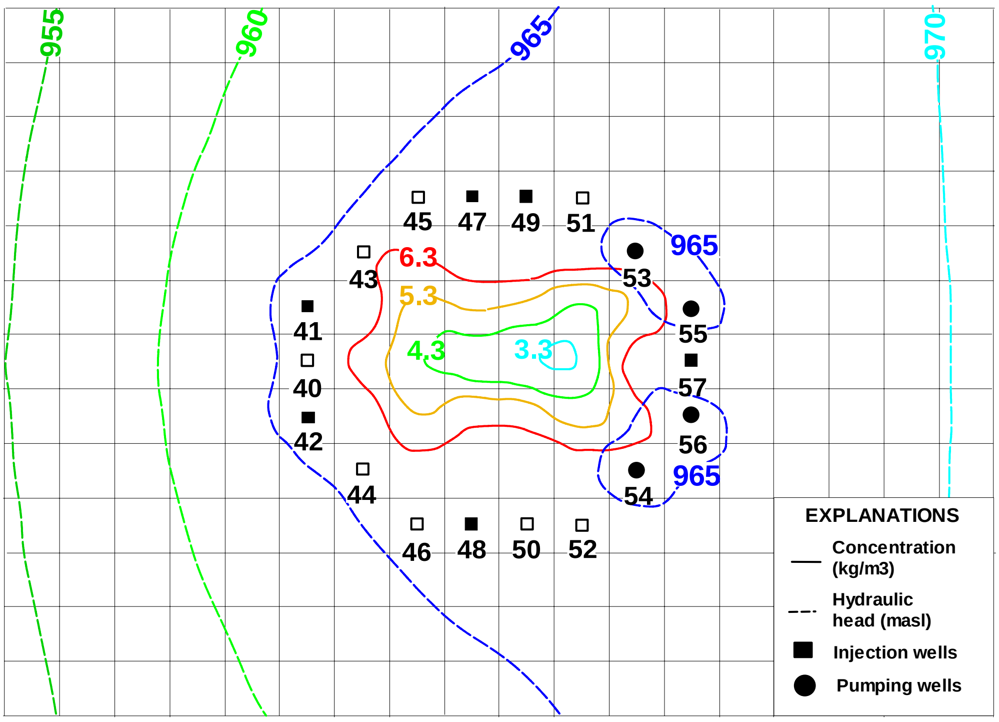


Fig. 6.19 Close-up view showing the fifth layer of the contained mound, injection and pumping wells for Case4 at the end of the planning period.

The optimal pumpage and injection rates are input back to the transient flow and transport model to check if the constraints are satisfied. The results show that the freshwater mound is held in its original location through the use of optimal hydraulic gradient control wells by creating a flat gradient around the freshwater mound boundary. The concentration and the hydraulic head distributions of the mound after the optimal schedules applied are presented in Figures 6.17, 6.18 and 6.19. Although; the hydraulic head values remain constant in the vertical direction throughout all the layers, the concentration values increase from the top layer to the bottom layer due to the density variations. Figures 6.20 and 6.21 show the vertical distributions of concentration and head values along a cross-section taken at y = 5100 m, respectively.

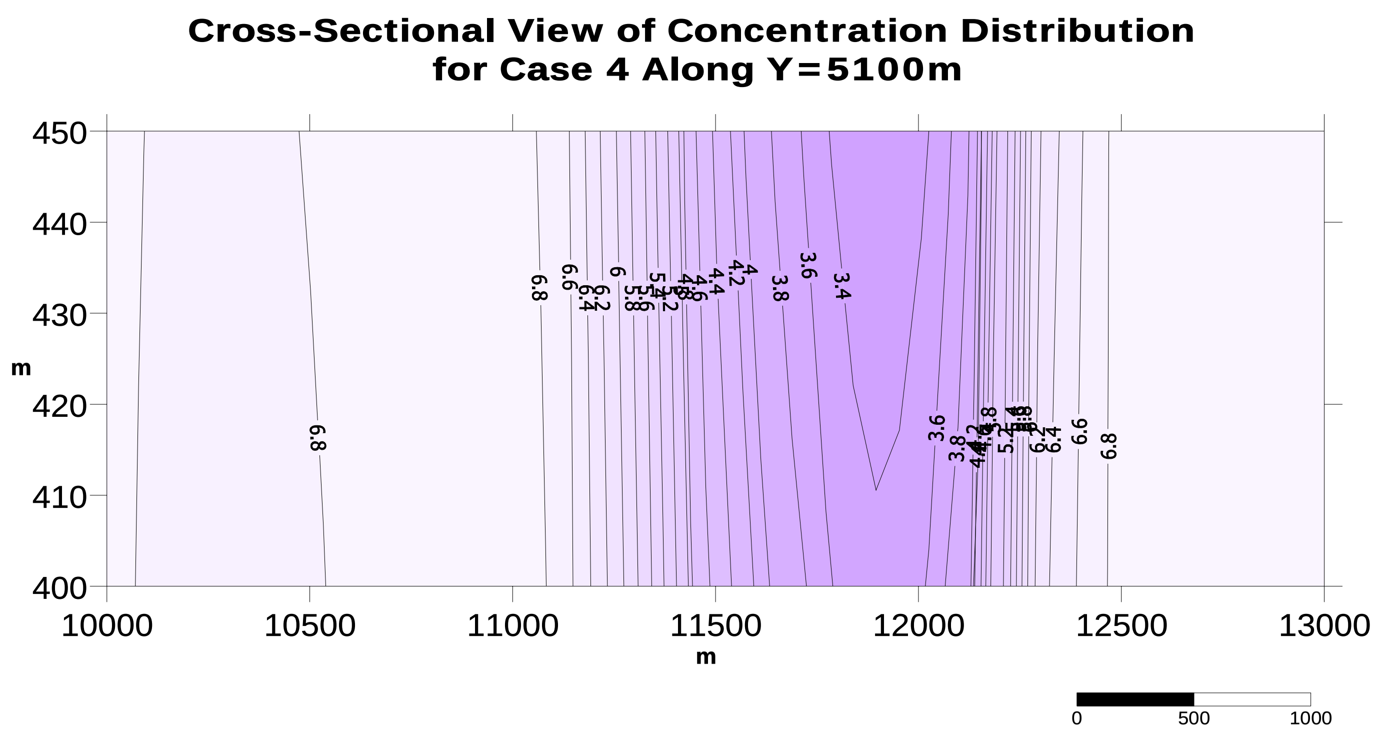


Fig. 6.20 Cross-sectional view of concentration distribution for Case 4 along y = 5100 m at the end of the planning period.

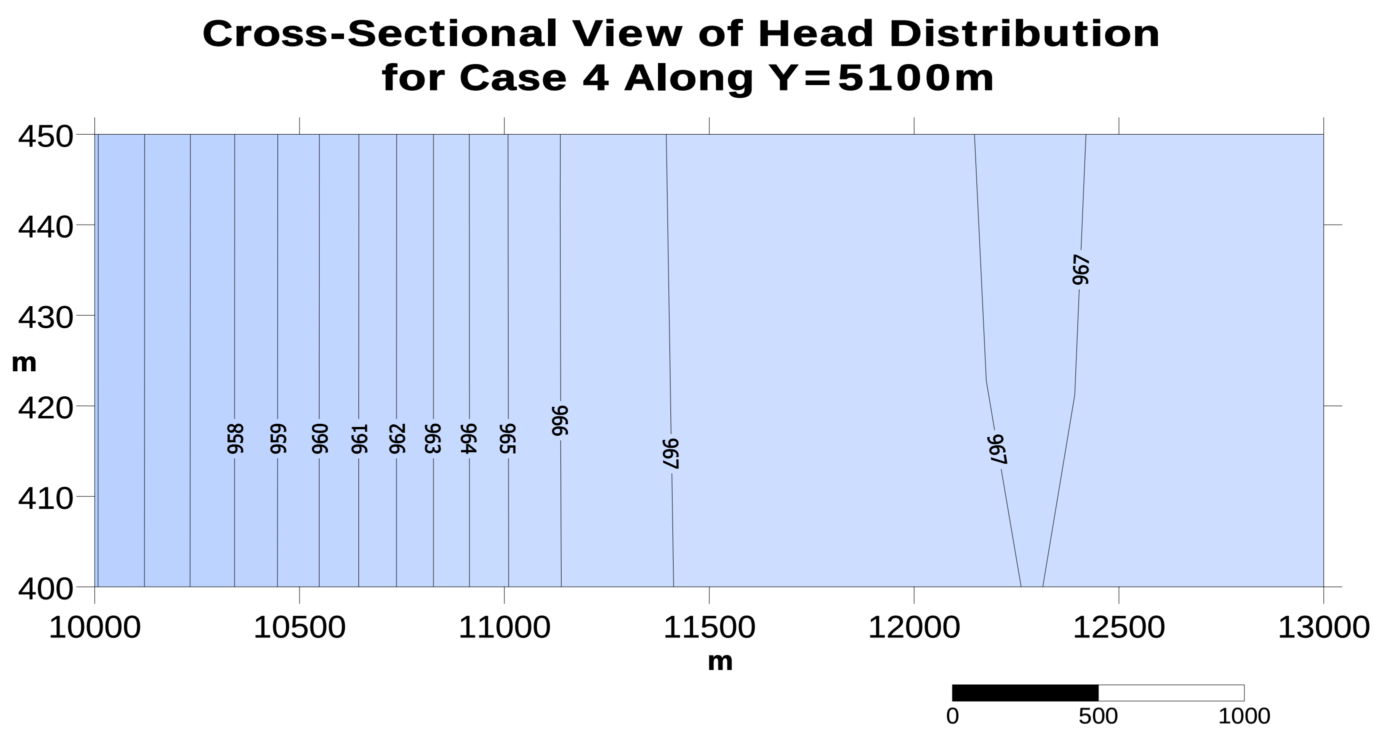


Fig. 6.21 Cross-sectional view of head distribution for Case 4 along y = 5100 m at the end of the planning period.

Different pumpage and injection rates associated with each well are shown in Figure 6.22. It can be seen from the charts that the major amount of the injected water is brought in from the 39th well. The others inject rather less water. The 41st, 42nd, and 57th wells may be left as unopened because they operate only in few time steps and inject very small amounts of water. Then again, the 20th, 53rd, and 55th wells operate at a minimum among the pumping wells hence they may be deactivated if economic priorities are taken into consideration. The total pumpage from the pumping wells is 8.26 $m^3 s^{-1}$ whereas the total injection amount is 8.81 $m^3 s^{-1}$. They add up to 17.07 $m^3 s^{-1}$ in total. The demand amount is not considered in the objective value. It is supplied from the water supply wells and equals 2.03 $m^3 s^{-1}$ which makes a total of 10.29 $m^3 s^{-1}$ verifying that the fourth constraint explained in Chapter 5 is satisfied.

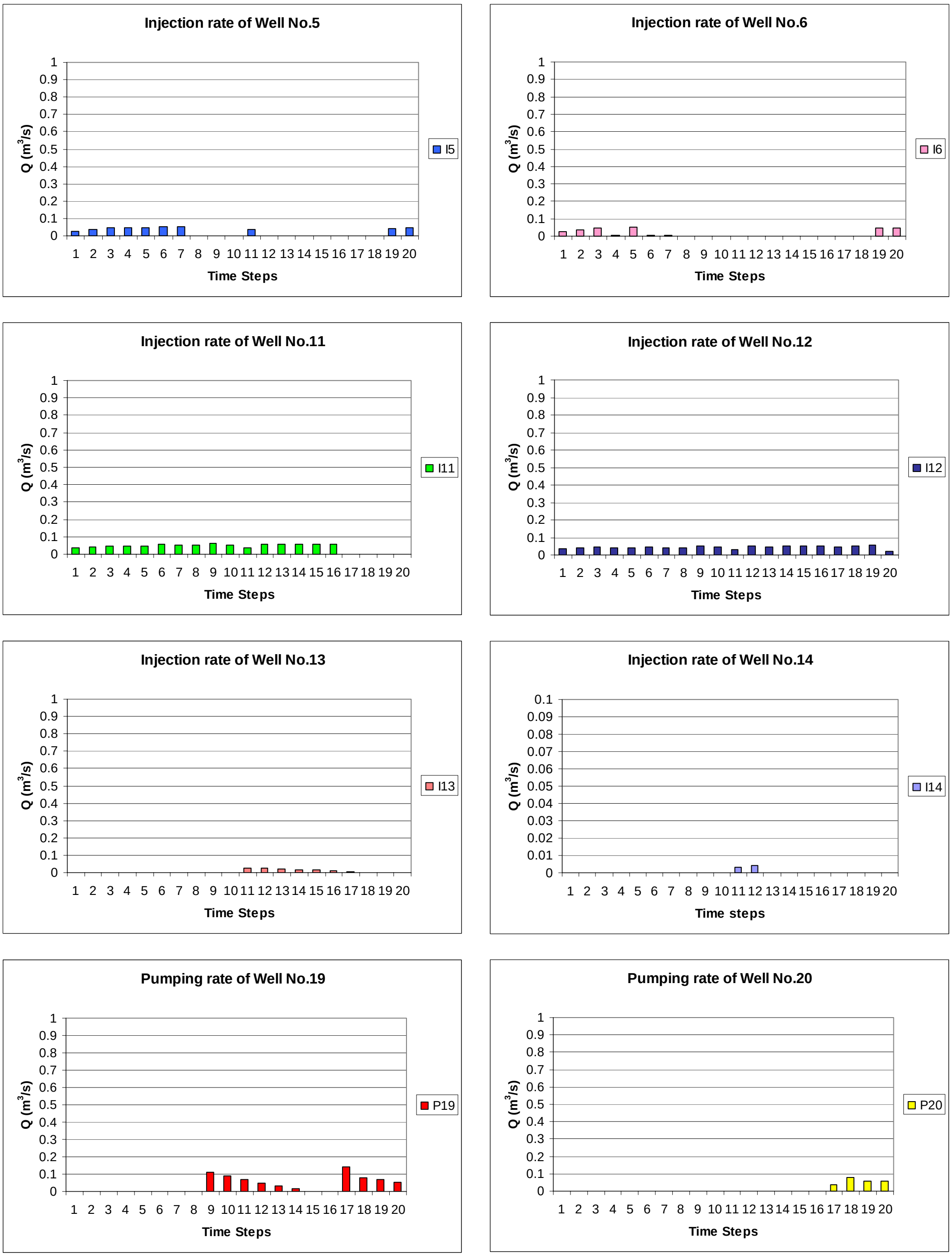


Fig. 6.22 Optimal injection and pumping schedules obtained from the optimization model Case4.

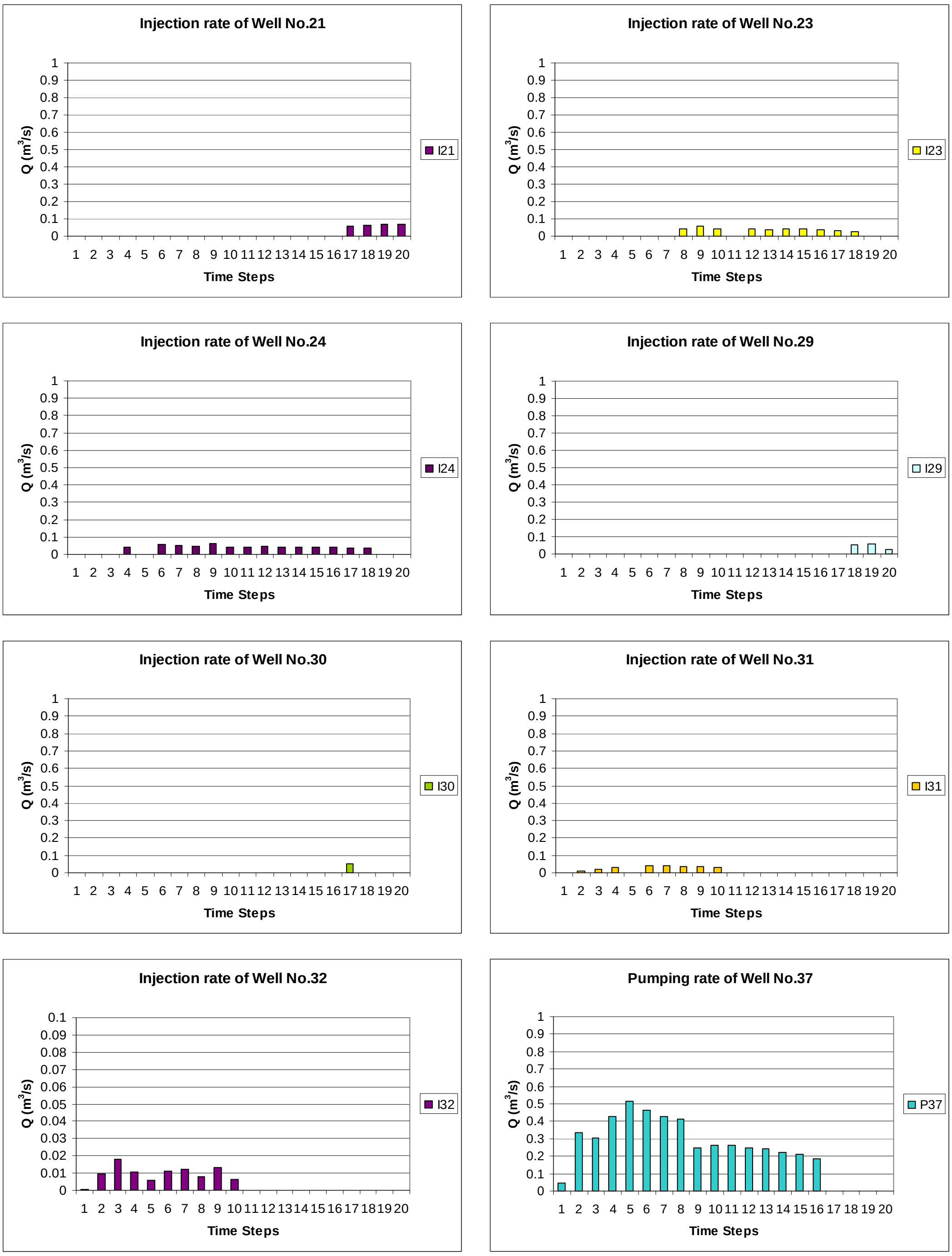


Fig. 6.22 (Continued)

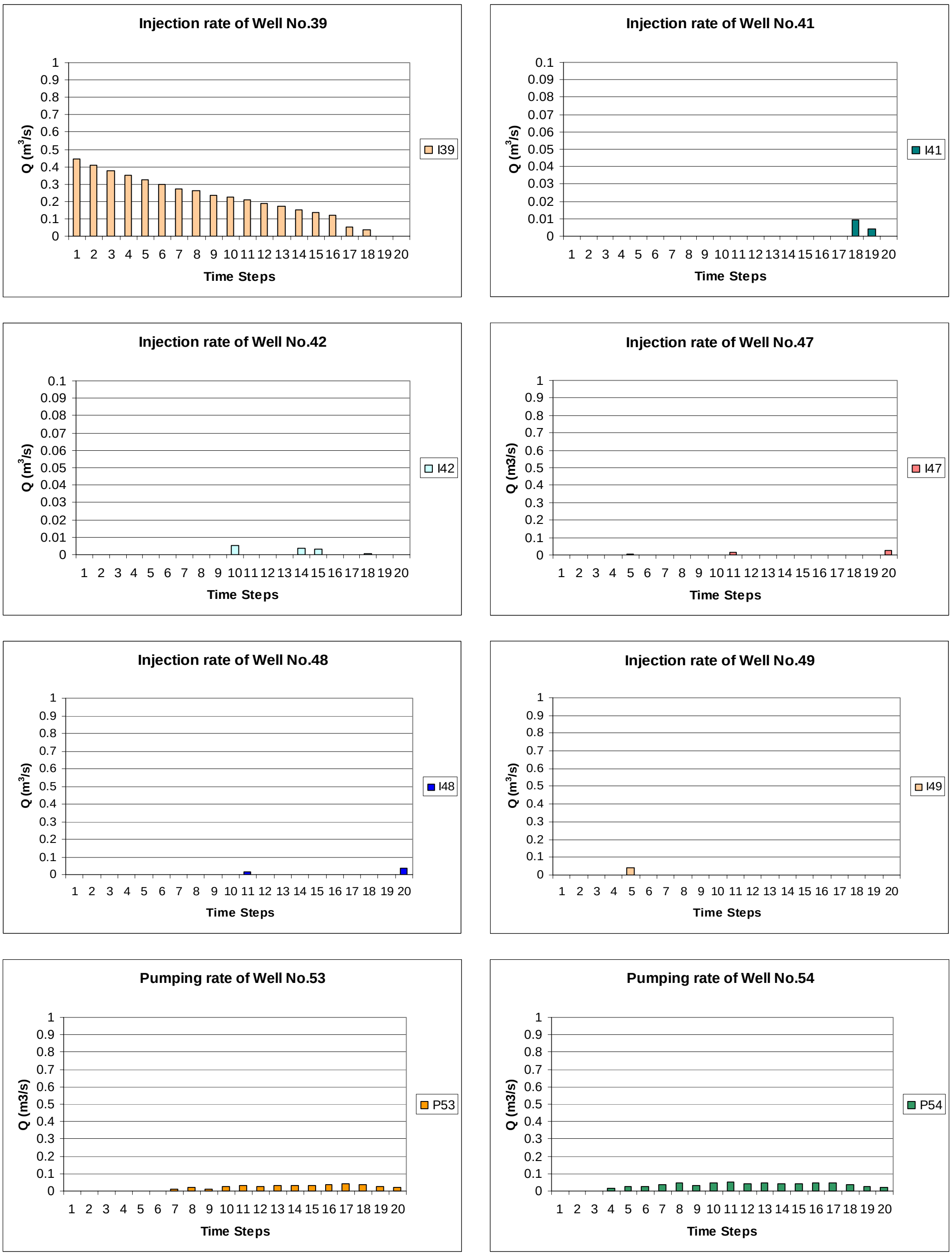
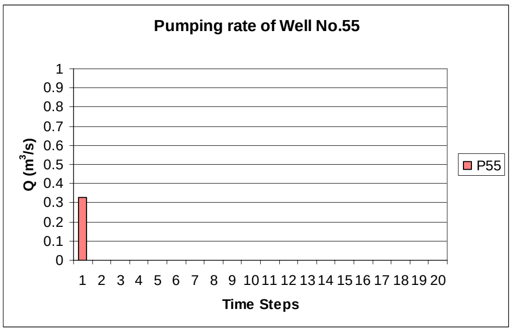
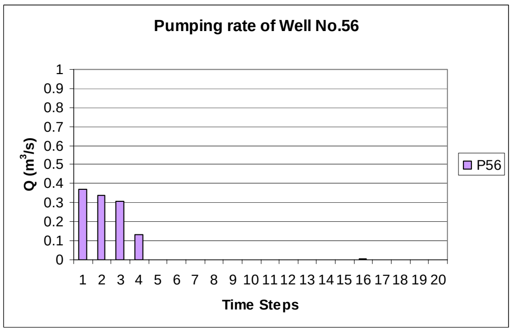


Fig. 6.22 (Continued)





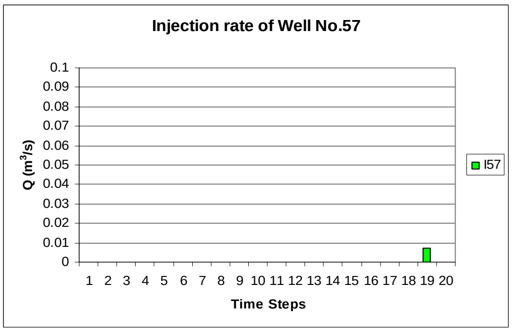


Fig. 6.22 (Continued)

Figure 6.23 shows the pumping and injection rates according to the time steps for Case 4. While the demand increases seasonally, the pumping and injection rates decrease significantly towards the end of the planning period. This decreasing behavior of pumping and injection wells is the opposite of the behavior of pumping and injection wells in Case 1 and Case 2.

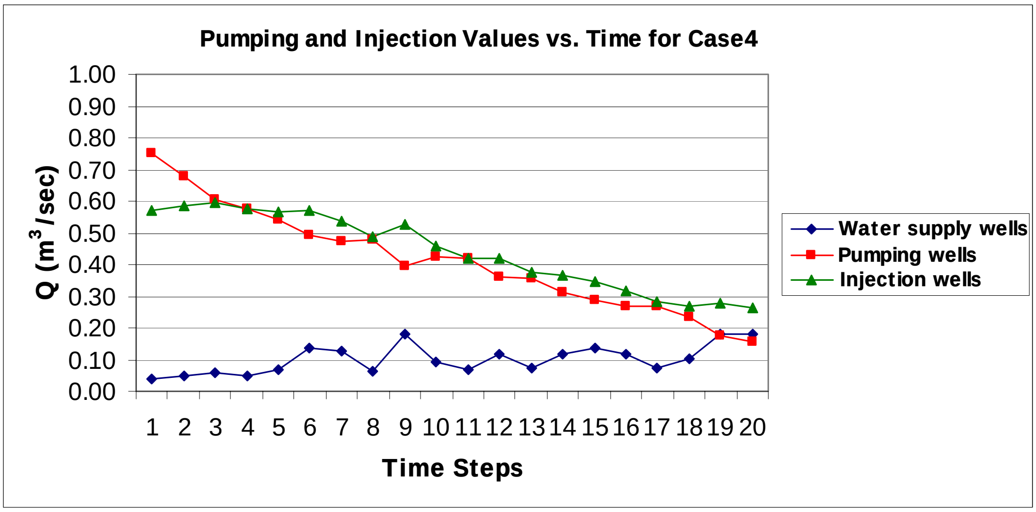


Fig. 6.23 Pumping and injection rates versus time for Case4 during the whole planning period.

The same model is solved again with upper bounds of 60 L s^{-1} on pumping and injection wells and an objective function value of 17.42 L s^{-1} is obtained. According to that solution, the 9th, 10th, 19th, 20th wells at the first layer (Fig. 6.24), the 25th, 27th, 28th, 37th, 38th wells at the third layer (Fig. 6.25), and the 43rd, 45th, 46th, 53rd, 54th, 55th, 56th wells at the fifth layer (Fig. 6.26) are utilized as pumping wells. On the other hand, the 4th, 5th, 6th, 11th, 12th, 13th, 14th, 15th, 16th, and 21st wells at the first layer (Fig. 6.24), the 22nd, 23rd, 24th, 29th, 30th, 31st, 32nd, 33rd, 39th wells at the third layer (Fig. 6.25), and the 41st, 42nd, 47th, 48th, 52nd, and 57th wells at the fifth layer (Fig. 6.26) are operated as injection wells.

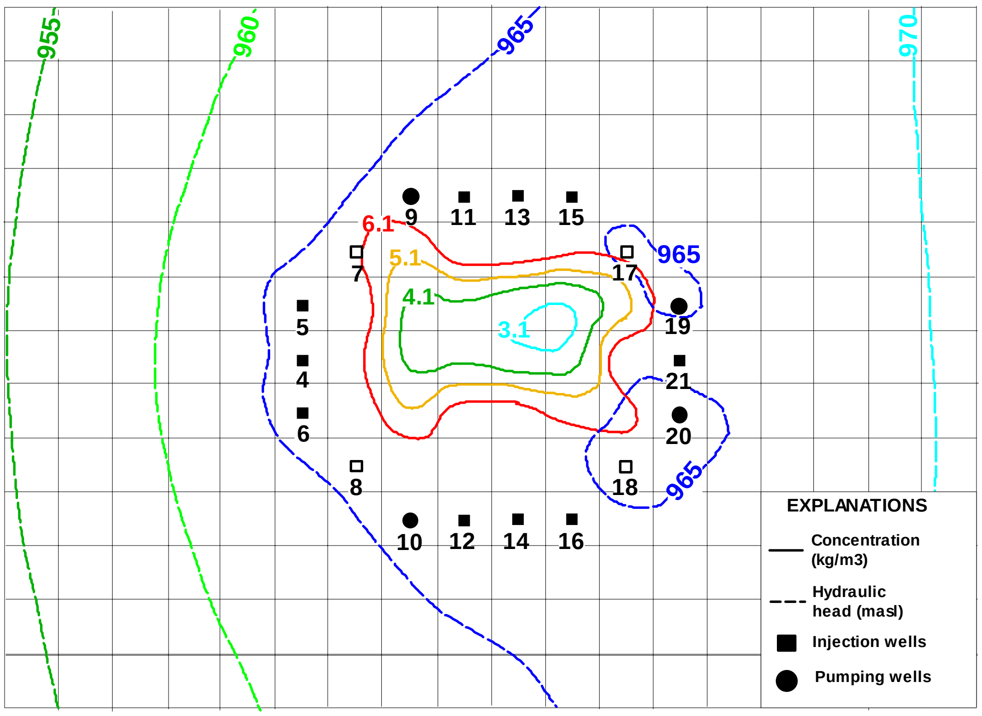


Fig 6.24 Close-up view showing the first layer of the contained mound, injection and pumping wells for Case4 at the end of the planning period when the upper bounds of 60 L s^{-1} are applied.

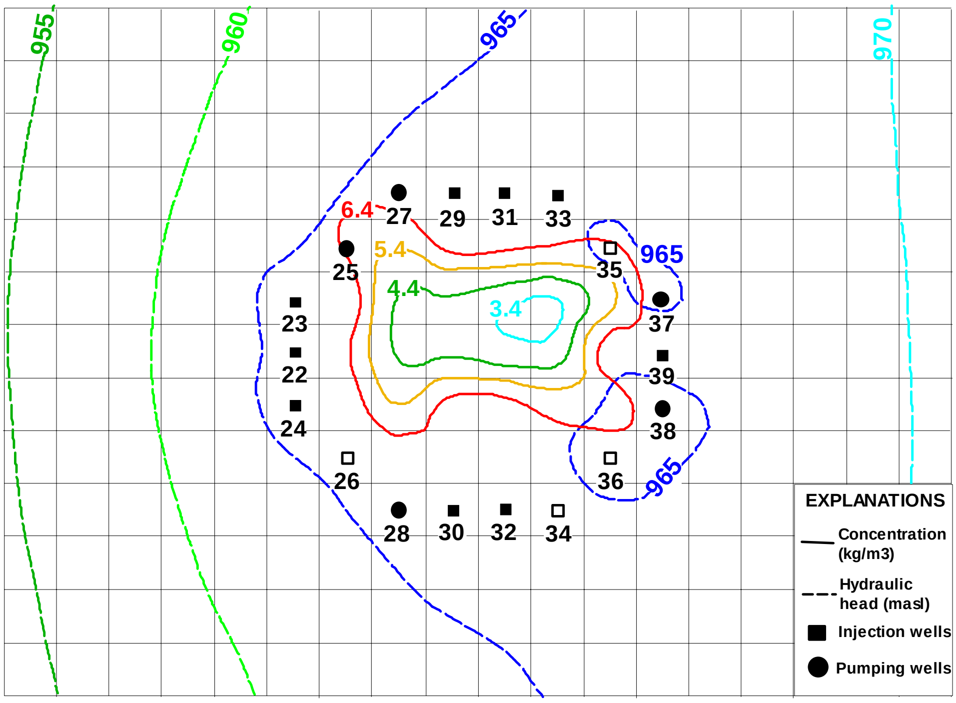


Fig 6.25 Close-up view showing the third layer of the contained mound, injection and pumping wells for Case4 at the end of the planning period when the upper bounds of 60 L s^{-1} are applied.

The optimal pumpage and injection rates are input back to the transient flow and transport model to check if the constraints are satisfied. The freshwater mound is kept from migration through the use of optimal hydraulic gradient control wells by creating a flat gradient around the freshwater mound boundary. The concentration and the hydraulic head distributions of the mound after the optimal schedules applied are presented in Figures 6.24, 6.25 and 6.26. The figures show that the optimal solution has selected to operate more wells than the optimal solution of the case without upper bounds. Then again, the hydraulic head values remain constant in the vertical direction throughout all the layers, the concentration values increase from the top layer to the bottom layer due to the density variations.

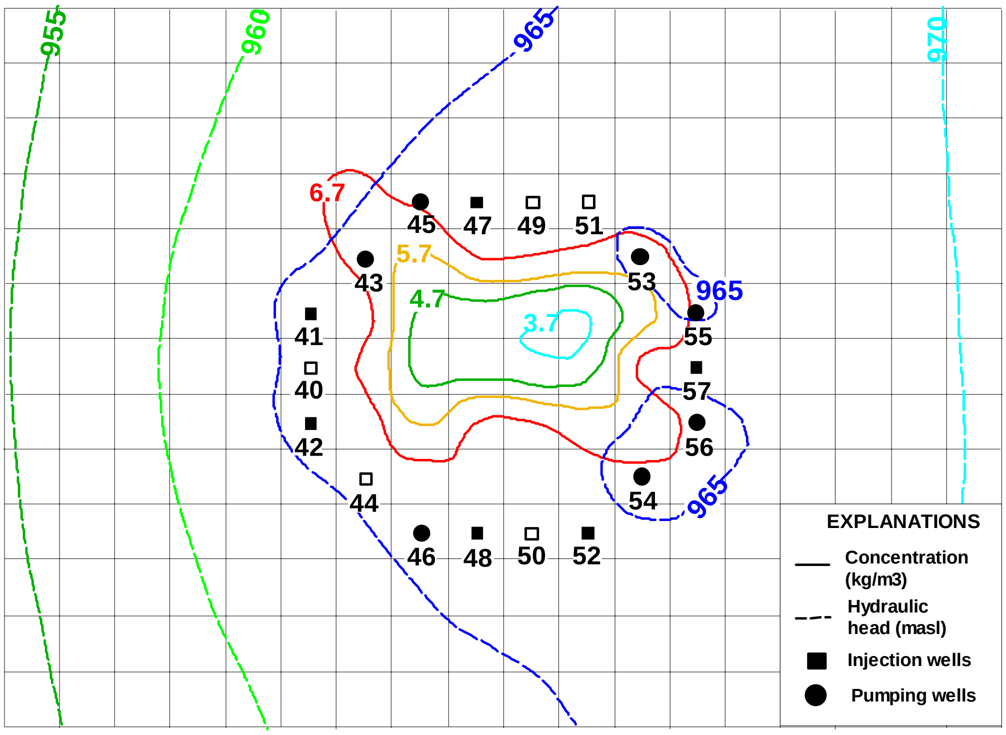


Fig 6.26 Close-up view showing the fifth layer of the contained mound, injection and pumping wells for Case4 at the end of the planning period when the upper bounds of 60 L s^{-1} are applied.

Different pumpage and injection rates associated with each well are shown in Figure 6.27. As it can be seen from the charts, the major amount of the pumping water is supplied from the 53rd well. The others pump rather less water and most of the pumping wells operate even only for one time step during the whole planning period. On the contrary, the most part of the injected water comes from the 11th, 23rd, 24th, 29th, 30th, 39th, 48th, and 57th wells which may be considered as the main injection wells among the others. The total pumpage from the pumping wells is 8.05 m^3 s^{-1} whereas the total injection amount is 9.37 m^3 s^{-1}. They add up to 17.42 m^3 s^{-1} in total. The demand amount is supplied from the water supply wells and is not considered in the objective value. It is 2.67 m^3 s^{-1}

making a total of 10.72 $m^3 s^{-1}$ which proves that the fourth constraint explained in Chapter 5 is satisfied.

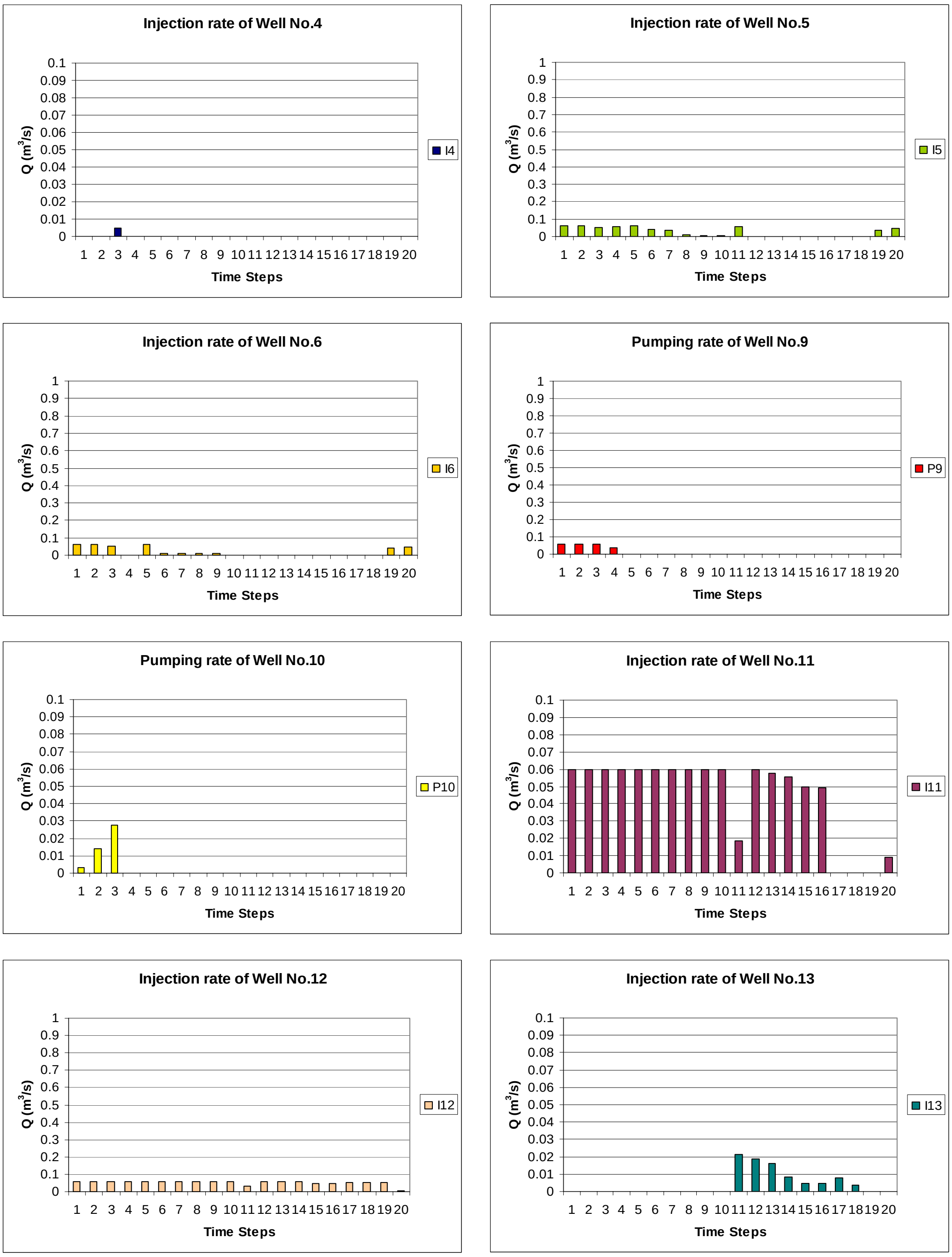


Fig. 6.27 Optimal injection and pumping schedules obtained from the optimization model Case4 when the upper bounds of 60 L s^{-1} are applied.

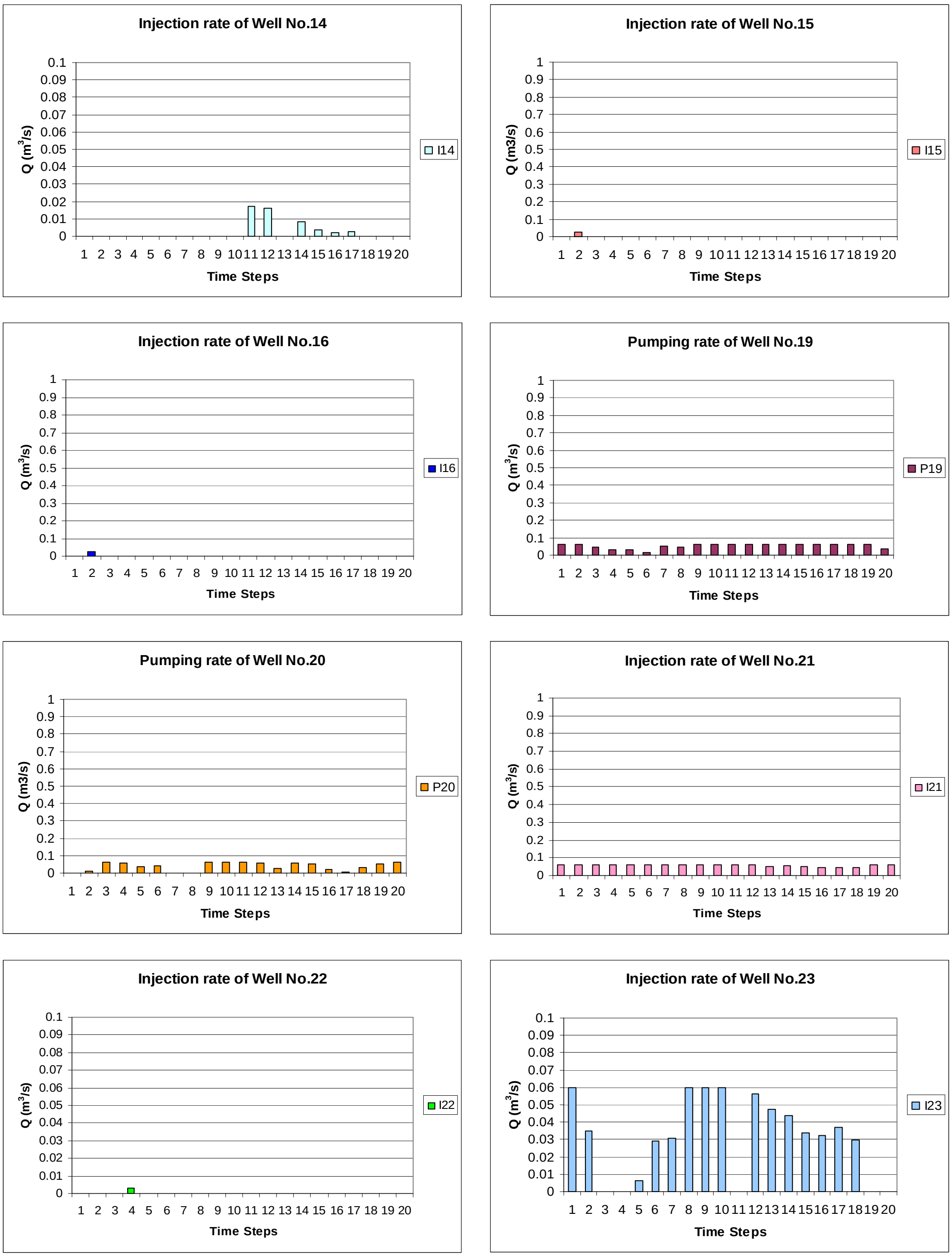


Fig. 6.27 (Continued)

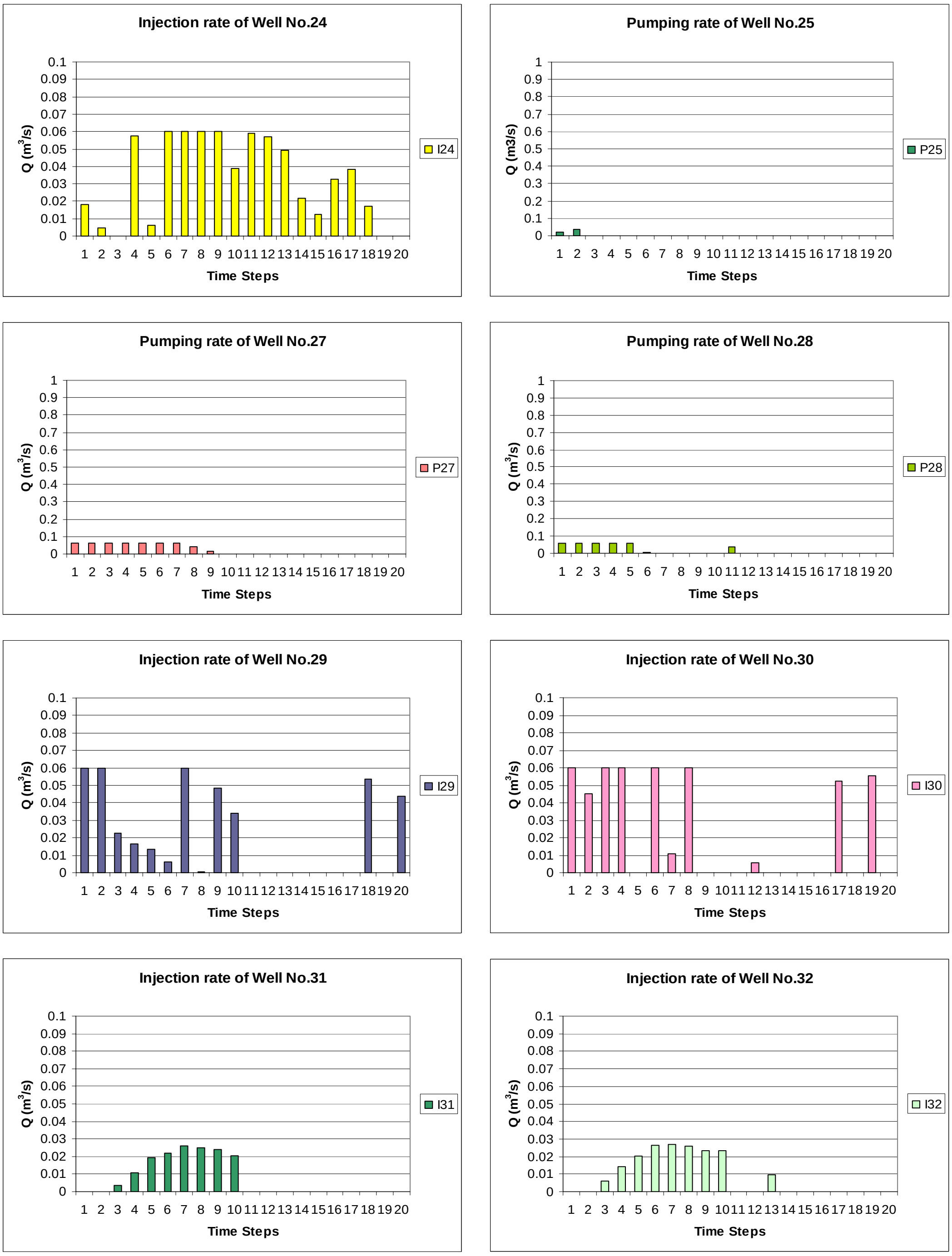


Fig. 6.27 (Continued)

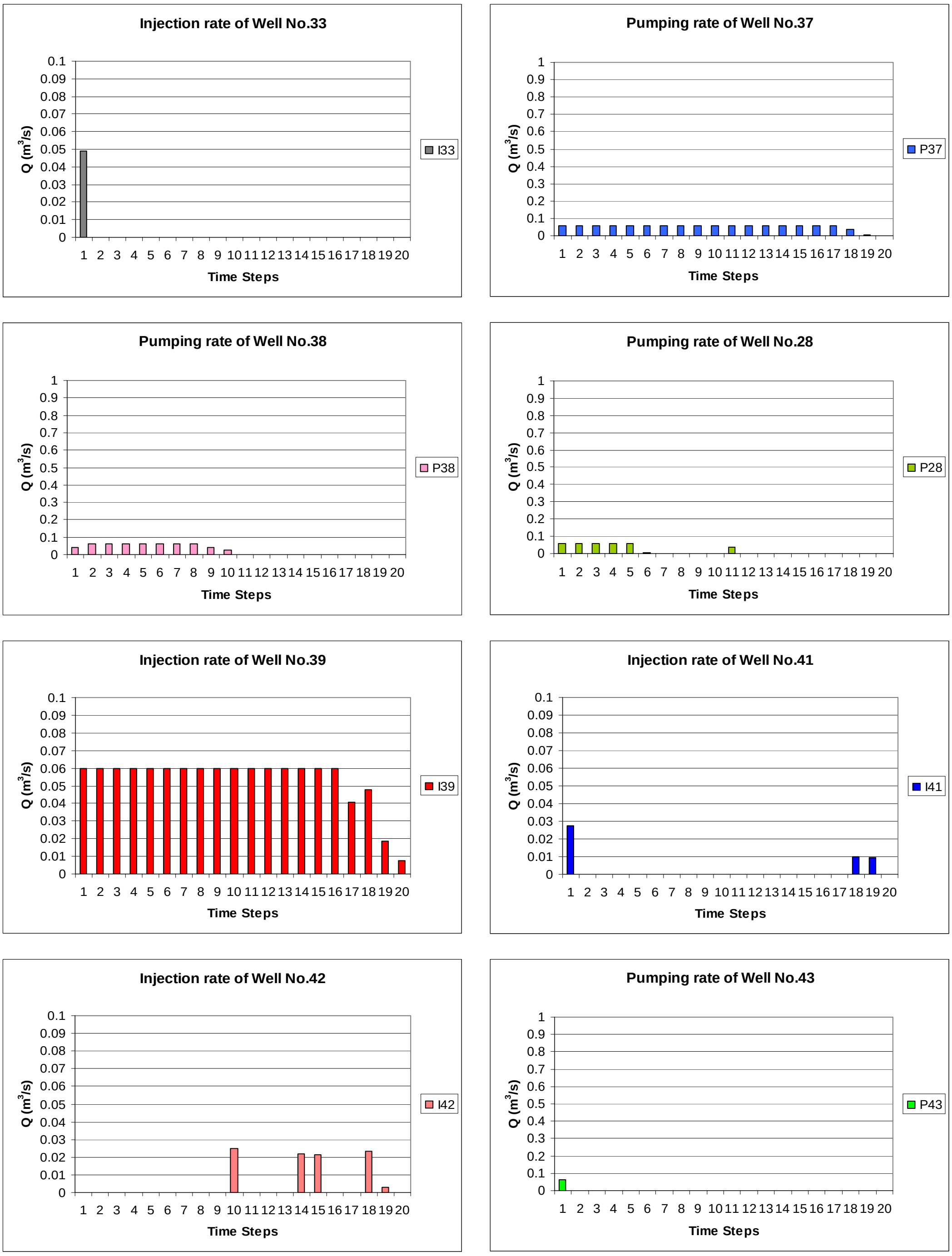


Fig. 6.27 (Continued)

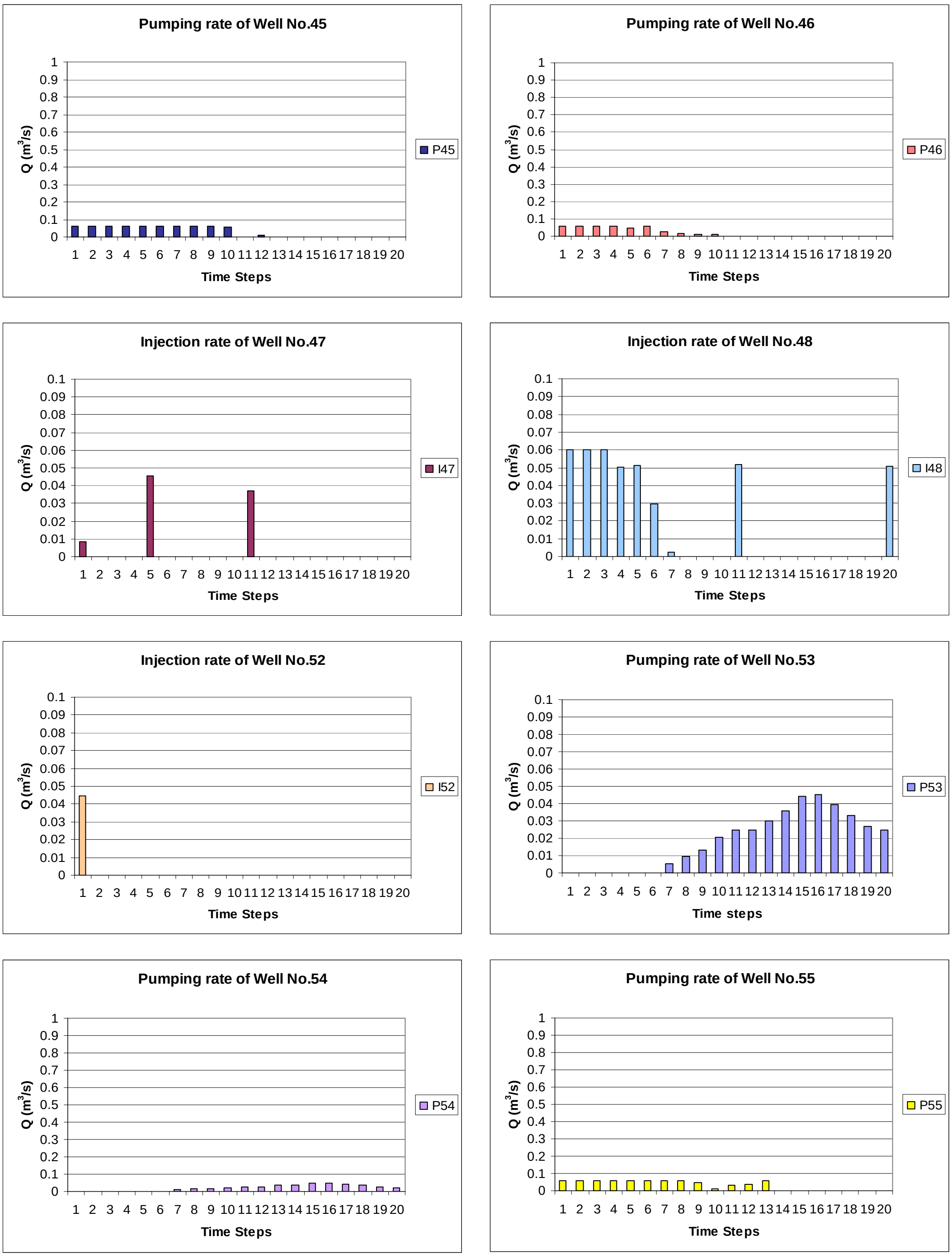
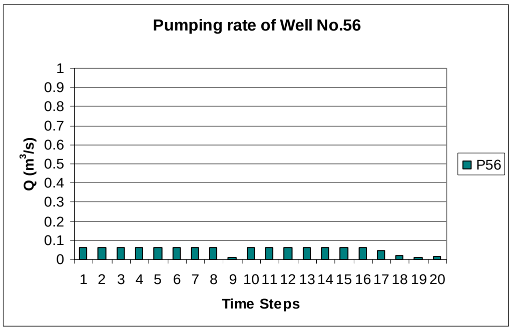


Fig. 6.27 (Continued)



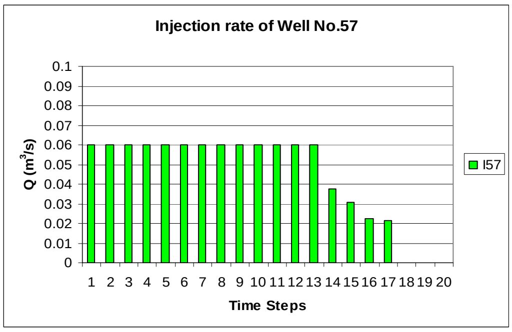


Fig. 6.27 (Continued)

Figure 6.28 shows the pumping and injection rates according to the time steps for Case 4 when the upper bounds of 60 L s^{-1} on pumping and injection wells are taken into account. It is clear from the figure that the demand amount and the pumping and injection rates show closer trends when compared with those of the Case 4 without any upper bounds. However, the optimal solution of the case with upper bounds opens much more wells and uses higher amounts of water when compared to the same case without the upper bounds. Therefore, the objective function value obtained by solving Case 4, free of any upper bounds is favored as a more feasible solution.

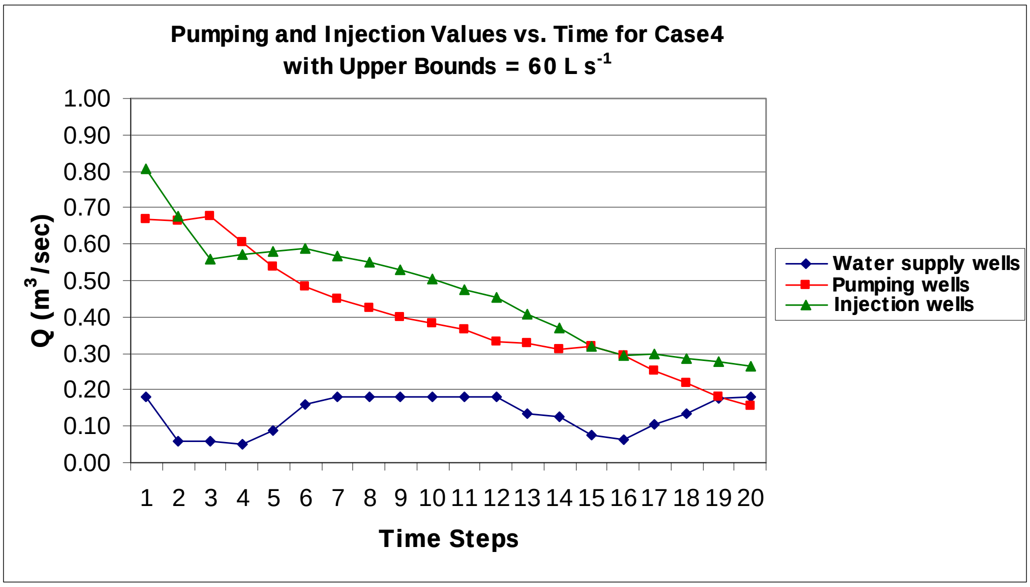


Fig. 6.28 Pumping and injection rates versus time for Case4 during the whole planning period when the upper bounds of 60 L s^{-1} are applied.

CHAPTER 7

SUMMARY&CONCLUSIONS

The process of freshwater storage in saline aquifers involves three steps which are injection of freshwater, storage and containment, and recovery of the stored water. This study focuses mainly on the second step.

In this study, the optimal storage and containment of a freshwater mound is formulated through the use of coupled simulation-optimization models that determine the best pumping/injection schedules both for constant density and variable density flows in single- and multi-layered aquifers. The models are applied to a hypothetical but realistic groundwater system. They are subject to constraints related with the;

1) satisfaction of the water demand requirements for each planning period,
2) satisfaction of the drawdown/build-up response equations,
3) reversal of gradient at control pairs,
4) restriction on total injection rate must not exceed total pumping rate,
5) restrictions upon maximum and minimum allowable injection and pumping rates.

The storage and containment of freshwater is tested for four different types of flow and aquifer conditions such as constant-density flow in a single-layered aquifer, constant-density flow in a multi-layered aquifer, variable-density flow in a single-layered aquifer, and variable-density flow in a multi-layered aquifer. The optimal solutions of the four different groundwater systems are obtained and evaluated on the basis of minimizing the sum of pumping and injection rates of hydraulic gradient control wells.

Conclusions from this study can be withdrawn as:

1) All of the proposed models are capable of retaining the freshwater mound from migrating down-gradient by means of hydraulic gradient control pairs which create inward or zero gradients at the mound boundary while satisfying the constraints they are subject to.

2) The results obtained from the applications of the models to the constant-density flow show that the hydraulic head and concentration does not show variations in the vertical direction. They remain constant even if the aquifer is multi-layered.

3) The results obtained from the applications of the models to the variable-density flow show that the hydraulic head and concentration does show variations in the vertical direction. They increase as the depth increases.

4) The results obtained from the applications of the models to the constant-density flow for single-layered and multi-layered aquifers show that, the optimal objective values are independent of whether upper bounds on pumping and injection wells are imposed or not.

5) The results obtained from the applications of the models to the variable-density flow for single-layered and multi-layered aquifers show that, the optimal objective values are dependent on the upper bounds imposed on pumping and injection wells.

6) The optimal objective values obtained by assuming constant-density flow for the one- and five-layered aquifers are equal to each other

signifying that the layering of the aquifer does not have any effect on the optimal solution in the case of constant-density flow.

7) The optimal objective value obtained by assuming variable-density flow for the five-layered aquifer is less than that of the one-layered aquifer confirming the fact that the density variations affect the flow field more significantly as the depth increases.

8) The results show that the process of optimal storage and containment of freshwater becomes less complex and more economical when the density effects are ignored.

9) The storage and containment of freshwater in optimal manners provides an alternative source for water supply during the times of droughts or emergencies.

10) For future studies, it is recommended that a sensitivity analysis demonstrating the effects of the aquifer parameters on the optimal objective policy should be performed.

11) Finally, this work showed that that the simulation of variable-density flow and understanding its effects on groundwater systems can be challenging and there is still a lot to discover in the world of variable-density phenomenon.

Above all the conclusions, the significant difference between the optimal solutions of constant-density and variable-density flow systems is noteworthy. The reason of this notable difference may be due to the possibility that the variable-density flow causes an aquifer system to behave as a non-linear system, which, in that case, will lead to the application of response function approach ineffective. Therefore, the linearity of the system should be checked in order to figure out if the response function approach will work properly or not in a groundwater system with variable-density flow before applying any linearization techniques.

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APPENDIX A

LISTING OF THE MPS GENERATION PROGRAM FOR THE CONSTANT-AND VARIABLE-DENSITY FLOWS IN SINGLE-LAYERED AQUIFER SYSTEMS

```
***************************************************************
C LP MATRIX GENERATOR IN MPS FORMAT
***************************************************************
      COMMON /C01/ BETA(30,45,20)
      COMMON /C02/ NPW,NOBW,NTS,NPAIR,NIW,NTW
      COMMON /C03/ UPBQ(30),SMAX(45),QMIN(30),QTOT
      COMMON /C04/ ITITLE(2),HI(45,20)
      COMMON /C05/ QLB(30,20)
      DIMENSION IIO(45),JJO(45),KKO(45)
      OPEN(5,FILE='injqin.dat')
      OPEN(6,FILE='ekran.dat')
      OPEN(8,FILE='pinq2.mps')
      OPEN(9,FILE='pinq2.spc')
      READ(5,5000) ITITLE
 5000 FORMAT(2A4)
      WRITE(6,6000) ITITLE
 6000 FORMAT(40X,2A4,/)
C
C. READ IN PLANNING PERIOD,NUMBER OF SEASONS,NUMBER OF WELLS,
ETC.
C
      READ(5,26) NOBW,NTS,NPAIR,NPW,NIW
   26 FORMAT(5I5)
C
C. READ IN TIME FACTOR IN SECONDS
C
      READ(5,222) STIME
      WRITE(6,222) STIME
  222 FORMAT(F10.0)
      WRITE(6,38)
   38 FORMAT(1H1,50X,'BETAS(SEC/MT**2)'//)
C
C. READ IN RESPONSE MATRIX(SEC/MT**2)
C
      NTW=NPW+NIW
      DO 1 I=1,NTW
      DO 1 K=1,NTS
      READ(5,27) (BETA(I,J,K),J=1,NOBW)
      IF(I.GT.NPW) GO TO 475
```

```
      DO 81 N=1,NOBW
      IF(BETA(I,N,K).LT.0.0) BETA(I,N,K)=0.0
   81 CONTINUE
      GO TO 18
 475  DO 82 N=1,NOBW
      IF(BETA(I,N,K).GT.0.0) BETA(I,N,K)=0.0
   82 CONTINUE
   18 WRITE(6,27)(BETA(I,J,K),J=1,NOBW)
    1 CONTINUE
C
C. READ TOTAL WATER REQUIRED(MT**3/SEC) DURING THE PLANNING
PERIOD
C
      READ(5,30) QTOT
      WRITE(6,31)QTOT
   30 FORMAT(F10.0)
   31 FORMAT(F10.3)
C
C. READ IN INDICES OF DRAWDOWN OBSERVATION WELLS
C
      READ(5,66) (IIO(K),JJO(K),K=1,NOBW)
      WRITE(6,66) (IIO(K),JJO(K),K=1,NOBW)
   66 FORMAT(24I3)
C
C. READ IN UPPER BOUNDS OF PUMPAGE FOR EACH PUMPING/INJECTION
WELL
C
      READ(5,99) (UPBQ(K),K=1,NTW)
      WRITE(6,98) (UPBQ(K),K=1,NTW)
   99 FORMAT(10F5.0)
   98 FORMAT(10F5.2)
C
C. READ IN LOWER BOUND OF PUMPAGE FOR EACH TIME STEP FOR EACH
WELL
C
      DO 55 IT=1,NTS
      READ(5,43) (QLB(K,IT),K=1,NTW)
      WRITE(6,433) (QLB(K,IT),K=1,NTW)
   43 FORMAT(8F8.0)
  433 FORMAT(8F8.3)
   55 CONTINUE
C
C. READ IN LOWER BOUND OF PUMPAGE FOR EACH TIME STEP FOR THE
AREA
C
      READ(5,40) (QMIN(IT),IT=1,NTS)
      WRITE(6,41) (QMIN(IT),IT=1,NTS)
   40 FORMAT(10F8.0)
   41 FORMAT(7F8.3)
C
C. READ IN UPPER BOUNDS TO DRAWDOWNS(MT) AT EACH DESIRED
LOCATION
C
      READ(5,45) (SMAX(K),K=1,NOBW)
      WRITE(6,451) (SMAX(K),K=1,NOBW)
   45 FORMAT(8F8.0)
  451 FORMAT(8F8.2)
```

```
C.
C. READ UNMANAGED HEADS AT DESIRED LOCATIONS AT EACH TIME
C.
      DO 88 IT=1,NTS
      READ(5,27) (HI(K,IT),K=1,NOBW)
C     WRITE(6,453) (HI(K,IT),K=1,NOBW)
C 452 FORMAT(6F10.0)
  453 FORMAT(6F10.2)
   88 CONTINUE
C
C. WRITE SECTION
C
      WRITE(6,33) NPW,NOBW
   33 FORMAT(//' NUMBER OF PUMPING WELLS =',I3,/' NUMBER OF
     1OBSERVATION WELLS =',I3/)
      WRITE(6,39) STIME
   39 FORMAT(' SCALING TIME FACTOR FOR BETAS =',F12.1,'
SECONDS')
      WRITE(6,300) QTOT
  300 FORMAT(' TOTAL WATER DEMAND FOR THE PLANNING PERIOD
=',F10.4)
      WRITE(6,207) (QMIN(IT),IT=1,NTS)
  207 FORMAT(5X,'LOWER LIMIT OF PUMPAGE FOR AREA DURING EACH
     1 TIME STEP',/10F8.4)
      WRITE(6,208) (IIO(K),JJO(K),K=1,NOBW)
  208 FORMAT(5X,'INDICES OF DRAWDOWN OBSERVATION WELLS',/,
     124I3)
      WRITE(6,210) (K,SMAX(K),K=1,NOBW)
  210 FORMAT(//,' MAXIMUM DRAWDOWN OF OBSERVATIN WELLS',//5X,
     1'OBSERVATION WELL',5X,' DRAWDOWN (MT)'/(5X,I4,15X,F7.2))
C  28 FORMAT( //' BETA(',I2,',J,',I2,')'/(8E15.5))
   27 FORMAT(5E15.5)
      WRITE(6,225) (IT,IT=1,NTS)
  225 FORMAT('1',2X,'MIN REQUIRED PUMP FOR EACH TIME STEP FOR
     1EACH PUMP WELL',//,2X,'WELL',10I7,/)
      DO 400 K=1,NPW
  400 WRITE(6,301) K,(QLB(K,IT),IT=1,NTS)
  301 FORMAT(I5,3X,10F7.3)
      CALL MATGEN
      STOP
      END
      SUBROUTINE MATGEN
C
C  *** THIS SUBROUTINE GENERATES THE LP MATRIX IN MPS FORMAT ***
C
      COMMON /C01/ BETA(30,45,20)
      COMMON /C02/ NPW,NOBW,NTS,NPAIR,NIW,NTW
      COMMON /C03/ UPBQ(30),SMAX(45),QMIN(30),QTOT
      COMMON /C04/ ITITLE(2),HI(45,20)
      COMMON /C05/ QLB(30,20)
C
C.GENERATE THE SPECS FILE
C ----------------------
      WRITE(9,3500) ITITLE
 3500 FORMAT('BEGIN',1X,2A4)
      WRITE(9,3001)
 3001 FORMAT(3X,'MINIMIZE')
```

```
      WRITE(9,3002)
 3002 FORMAT(3X,'OBJECTIVE MINQIW')
      WRITE(9,3003)
 3003 FORMAT(3X,'ROWS',6X,'2000')
      WRITE(9,3004)
 3004 FORMAT(3X,'COLUMNS',3X,'5000')
      WRITE(9,3005)
 3005 FORMAT(3X,'ELEMENTS',3X,'400000')
      WRITE(9,3105)
 3105 FORMAT(3X,'MPS FILE',3X,'10')
      WRITE(9,3006)
 3006 FORMAT(3X,'SCALE YES')
      WRITE(9,3007) ITITLE
 3007 FORMAT('END',1X,2A4)
C
C.GENERATE THE MPS FILE
C ---------------------
      WRITE(8,2008) ITITLE
 2008 FORMAT('NAME',T15,2A4)
      WRITE(8,2009)
 2009 FORMAT('ROWS')
C
C. SET UP ROW NAMES
C  ----------------
C.   1) TOTAL PUMPAGE FOR AREA FOR ALL TIME STEPS
C
      WRITE(8,2010)
 2010 FORMAT(1X,'G  TOTQ')
C
C.   2) TOTAL DEMAND FOR EACH TIME STEP
C
      DO 100 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2011) IT1,IT2
 2011 FORMAT(1X,'G  TQ',2I1)
  100 CONTINUE
C
C.   3) DRAWDOWN FOR EACH OBSERVATION WELL & EACH TIME STEP
C
      DO 105 IW=1,NOBW
      IW1=IW/10
      IW2=IW-IW1*10
      DO 105 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2012) IW1,IW2,IT1,IT2
 2012 FORMAT(1X,'E  D',4I1)
  105 CONTINUE
C
C.   4)  GRADIENT CONTROL CONSTRAINTS, C
C
      DO 115 IW=1,NPAIR
      IW1=IW/10
      IW2=IW-IW1*10
      DO 115 IT=1,NTS
      IT1=IT/10
```

```
      IT2=IT-IT1*10
      WRITE(8,2013) IW1,IW2,IT1,IT2
 2013 FORMAT(1X,'G  C',4I1)
  115 CONTINUE
C
C.   5) TOTAL INJECTION < TOTAL PUMPAGE FOR EACH TIME STEP
C
      DO 280 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2031) IT1,IT2
 2031 FORMAT(1X,'G  PI',2I1)
  280 CONTINUE
C
C.   6) OBJECTIVE FUNCTION NAME
C
      WRITE(8,2015)
 2015 FORMAT(1X,'N  MINQIW')
C
C.SET UP COEFFICIENTS OF COLUMNS
C  ------------------------------
      WRITE(8,2017)
 2017 FORMAT('COLUMNS')
C
C. ENTER COEFFICIENTS OF PUMPING RATES FOR DEMAND WELLS:
C
      DO 145 IW=1,NPW
      IW1=IW/10
      IW2=IW-IW1*10
      DO 145 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1) TOTQ EQUATION
C
      WRITE(8,2018) IW1,IW2,IT1,IT2
 2018 FORMAT('    Q',4I1,T15,'TOTQ',T25,'0.000001E+06')
C
C.                    2) TQ(T) EQUATION
C
      WRITE(8,2019) IW1,IW2,IT1,IT2,IT1,IT2
 2019 FORMAT('    Q',4I1,T15,'TQ',2I1,T25,'0.000001E+06')
C
C.                    3) PI(T) EQUATION
C
      WRITE(8,2059) IW1,IW2,IT1,IT2,IT1,IT2
 2059 FORMAT('    Q',4I1,T15,'PI',2I1,T25,'0.000001E+06')
C
C.                    4) DRAWDOWN D(W,T) EQUATIONS
C
      JJ=IW
      DO 140 II=1,NOBW
      IWW1=II/10
      IWW2=II-IWW1*10
      IS=IT
      KK=0
      DO 135 I=IS,NTS
```

```
      ITT1=I/10
      ITT2=I-ITT1*10
      KK=KK+1
      TAIJ=-BETA(JJ,II,KK)
      WRITE(8,2020) IW1,IW2,IT1,IT2,IWW1,IWW2,ITT1,ITT2,TAIJ
 2020 FORMAT('    Q',4I1,T15,'D',4I1,T25,E12.6)
  135 CONTINUE
  140 CONTINUE
C
C.                   5) OBJECTIVE FUNCTION COEFFICIENTS
C
      IF(IW.LE.NPW) GO TO 145
      WRITE(8,4020) IW1,IW2,IT1,IT2
 4020 FORMAT('    Q',4I1,T15,'MINQIW',T25,'0.000001E+06')
  145 CONTINUE
C
C. ENTER COEFFICIENTS OF PUMPING RATES FOR GRADIENT WELLS
C
      DO 445 IW=1,NIW
      IW1=IW/10
      IW2=IW-IW1*10
      DO 445 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1) PI(T) EQUATION
C
      WRITE(8,2061) IW1,IW2,IT1,IT2,IT1,IT2
 2061 FORMAT('    P',4I1,T15,'PI',2I1,T25,'0.000001E+06')
C
C.                    2) DRAWDOWN D(W,T) EQUATIONS
C
      JJ=NPW+IW
      DO 440 II=1,NOBW
      IWW1=II/10
      IWW2=II-IWW1*10
      IS=IT
      KK=0
      DO 435 I=IS,NTS
      ITT1=I/10
      ITT2=I-ITT1*10
      KK=KK+1
      TAIJ=BETA(JJ,II,KK)
      WRITE(8,7037) IW1,IW2,IT1,IT2,IWW1,IWW2,ITT1,ITT2,TAIJ
 7037 FORMAT('    P',4I1,T15,'D',4I1,T25,E12.6)
  435 CONTINUE
  440 CONTINUE
C
C.                   3) OBJECTIVE FUNCTION COEFFICIENTS
C
      WRITE(8,4120) IW1,IW2,IT1,IT2
 4120 FORMAT('    P',4I1,T15,'MINQIW',T25,'0.000001E+06')
  445 CONTINUE
C
C. ENTER COEFFICIENTS OF INJECTION RATES FOR GRADIENT WELLS
C
      DO 545 IW=1,NIW
```

```
      IW1=IW/10
      IW2=IW-IW1*10
      DO 545 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                   1) PI(T) EQUATION
C
      WRITE(8,2071) IW1,IW2,IT1,IT2,IT1,IT2
 2071 FORMAT('    I',4I1,T15,'PI',2I1,T25,'-0.00001E+05')
C
C.                   2) DRAWDOWN D(W,T) EQUATIONS
C
      JJ=NPW+IW
      DO 540 II=1,NOBW
      IWW1=II/10
      IWW2=II-IWW1*10
      IS=IT
      KK=0
      DO 535 I=IS,NTS
      ITT1=I/10
      ITT2=I-ITT1*10
      KK=KK+1
      TAIJ=-BETA(JJ,II,KK)
      WRITE(8,2120) IW1,IW2,IT1,IT2,IWW1,IWW2,ITT1,ITT2,TAIJ
 2120 FORMAT('    I',4I1,T15,'D',4I1,T25,E12.6)
  535 CONTINUE
  540 CONTINUE
C
C.                  3) OBJECTIVE FUNCTION COEFFICIENTS
C
      WRITE(8,4021) IW1,IW2,IT1,IT2
 4021 FORMAT('    I',4I1,T15,'MINQIW',T25,'0.000001E+06')
  545 CONTINUE
C
C. ENTER COEFFICIENTS OF S(W,T):
C
      DO 200 IW=1,NTW
      IW1=IW/10
      IW2=IW-IW1*10
      DO 200 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1) DRAWDOWN D(W,T) EQUATION
C
      WRITE(8,2050) IW1,IW2,IT1,IT2,IW1,IW2,IT1,IT2
 2050 FORMAT('    S',4I1,T15,'D',4I1,T25,'0.000001E+06')
  200 CONTINUE
      NSG=NTW+1
      KPAIR=2
      KK=1
      IC=1
C
C. ENTER COEFFICIENTS OF S(W,T) IN OTHER EQUATIONS
C
      TA=1.
```

```
      DO 500 IW=NSG,NOBW
      IW1=IW/10
      IW2=IW-IW1*10
      TB=-TA
      IC1=IC/10
      IC2=IC-IC1*10
      IF(KK.NE.KPAIR) GO TO 75
      KK=0
      IC=IC+1
   75 KK=KK+1
      DO 501 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1)DRAWDOWN EQUATIONS
C
      WRITE(8,2060) IW1,IW2,IT1,IT2,IW1,IW2,IT1,IT2
 2060 FORMAT('    S',4I1,T15,'D',4I1,T25,'0.000001E+06')
C
C.                    2) GRADIENT CONTROL EQUATIONS
C
      WRITE(8,2051) IW1,IW2,IT1,IT2,IC1,IC2,IT1,IT2,TB
 2051 FORMAT('    S',4I1,T15,'C',4I1,T25,E12.6)
  501 CONTINUE
      TA=-TA
  500 CONTINUE
C
C. ENTER COEFFICIENTS OF U(W,T):
C
      DO 220 IW=1,NTW
      IW1=IW/10
      IW2=IW-IW1*10
      DO 220 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1) DRAWDOWN D(W,T) EQUATION
C
      WRITE(8,2250) IW1,IW2,IT1,IT2,IW1,IW2,IT1,IT2
 2250 FORMAT('    U',4I1,T15,'D',4I1,T25,'-0.00001E+05')
  220 CONTINUE
      NSG=NTW+1
      KPAIR=2
      KK=1
      IC=1
C
C. ENTER COEFFICIENTS OF U(W,T) IN OTHER EQUATIONS
C
      TC=-1.
      DO 510 IW=NSG,NOBW
      IW1=IW/10
      IW2=IW-IW1*10
      TD=-TC
      IC1=IC/10
      IC2=IC-IC1*10
      IF(KK.NE.KPAIR) GO TO 76
      KK=0
```

```
      IC=IC+1
   76 KK=KK+1
      DO 601 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1)DRAWDOWN EQUATIONS
C
      WRITE(8,3061) IW1,IW2,IT1,IT2,IW1,IW2,IT1,IT2
 3061 FORMAT('    U',4I1,T15,'D',4I1,T25,'-0.00001E+05')
C
C.                    2) GRADIENT CONTROL EQUATIONS
C
      WRITE(8,3071) IW1,IW2,IT1,IT2,IC1,IC2,IT1,IT2,TD
 3071 FORMAT('    U',4I1,T15,'C',4I1,T25,E12.6)
  601 CONTINUE
      TC=-TC
  510 CONTINUE
C
C.SET UP RIGHT-HAND SIDE:
C ----------------------
C
      WRITE(8,2029)
 2029 FORMAT('RHS')
C
C.                    1) TOTQ EQUATION
C
      WRITE(8,2030) QTOT
 2030 FORMAT(T5,'RHS1',T15,'TOTQ',T25,F12.4)
C
C.                    2) TOTAL DEMAND FOR EACH TIME STEP
C
      DO 3000 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,7031) IT1,IT2,QMIN(IT)
 7031 FORMAT(T5,'RHS1',T15,'TQ',2I1,T25,E12.6)
 3000 CONTINUE
C
C. ENTER RHS OF GRADIENT CONTROL CONSTRAINTS
C
      JP=1
      DO 777 IC=1,NPAIR
      II1=NTW+JP
      II2=II1+1
      IC1=IC/10
      IC2=IC-IC1*10
      JP=JP+2
      DO 777 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      GRHS=HI(II2,IT)-HI(II1,IT)
      WRITE(8,778) IC1,IC2,IT1,IT2,GRHS
  778 FORMAT(T5,'RHS1',T15,'C',4I1,T25,E12.6)
  777 CONTINUE
C
C. ENTER RHS OF PI CONSTRAINTS SO THAT THEY ARE EQUAL TO DEMAND
```

```
C
      DO 3033 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      PIRHS=QMIN(IT)
      WRITE(8,7047) IT1,IT2,PIRHS
 7047 FORMAT(T5,'RHS1',T15,'PI',2I1,T25,E12.6)
 3033 CONTINUE
C
C. SET UP BOUNDS SECTION:
C  ---------------------
      WRITE(8,2034)
 2034 FORMAT('BOUNDS')
C
C.             1) LOWER & UPPER PUMPING LIMITS FOR DEMAND WELLS
C
      DO 175 IW=1,NPW
      IW1=IW/10
      IW2=IW-IW1*10
      DO 175 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2038) IW1,IW2,IT1,IT2,QLB(IW,IT)
 2038 FORMAT(' LO BOUND ',T15,'Q',4I1,T25,E12.6)
      WRITE(8,2035) IW1,IW2,IT1,IT2,UPBQ(IW)
 2035 FORMAT(' UP BOUND ',T15,'Q',4I1,T25,E12.6)
  175 CONTINUE
      DO 278 IW=1,NIW
      IW1=IW/10
      IW2=IW-IW1*10
      IK=NPW+IW
      DO 278 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,5035) IW1,IW2,IT1,IT2,UPBQ(IK)
 5035 FORMAT(' UP BOUND ',T15,'P',4I1,T25,E12.6)
      WRITE(8,5036) IW1,IW2,IT1,IT2,UPBQ(IK)
 5036 FORMAT(' UP BOUND ',T15,'I',4I1,T25,E12.6)
  278 CONTINUE
      WRITE(8,2036)
 2036 FORMAT('ENDATA')
      WRITE(6,2037)
 2037 FORMAT(5X,'**** MATRIX FOR LP IS GENERATED ON UNIT 8
****')
      RETURN
      END
```

APPENDIX B

LISTING OF THE MPS GENERATION PROGRAM FOR THE CONSTANT- AND VARIABLE-DENSITY FLOWS IN MULTI-LAYERED AQUIFER SYSTEMS

```
**************************************************************
C LP MATRIX GENERATOR IN MPS FORMAT
***************************************************************
      COMMON /C01/ BETA(60,120,20)
      COMMON /C02/ NPW,NOBW,NTS,NPAIR,NIW,NTW
      COMMON /C03/ UPBQ(60),SMAX(120),QMIN(60),QTOT
      COMMON /C04/ ITITLE(2),HI(120,20)
      COMMON /C05/ QLB(60,20)
      DIMENSION IIO(120),JJO(120),KKO(120)
      OPEN(5,FILE='injqin.dat')
      OPEN(6,FILE='ekran.dat')
      OPEN(8,FILE='pinq2.mps')
      OPEN(9,FILE='pinq2.spc')
      READ(5,5000) ITITLE
 5000 FORMAT(2A4)
      WRITE(6,6000) ITITLE
 6000 FORMAT(40X,2A4,/)
C
C. READ IN PLANNING PERIOD,NUMBER OF SEASONS,NUMBER OF WELLS,
ETC.
C
      READ(5,26) NOBW,NTS,NPAIR,NPW,NIW
   26 FORMAT(5I5)
C
C. READ IN TIME FACTOR IN SECONDS
C
      READ(5,222) STIME
      WRITE(6,222) STIME
  222 FORMAT(F10.0)
      WRITE(6,38)
   38 FORMAT(1H1,50X,'BETAS(SEC/MT**2)'//)
C
C. READ IN RESPONSE MATRIX(SEC/MT**2)
C
      NTW=NPW+NIW
      DO 1 I=1,NTW
      DO 1 K=1,NTS
      READ(5,27) (BETA(I,J,K),J=1,NOBW)
      IF(I.GT.NPW) GO TO 475
```

```
      DO 81 N=1,NOBW
      IF(BETA(I,N,K).LT.0.0) BETA(I,N,K)=0.0
   81 CONTINUE
      GO TO 18
  475 DO 82 N=1,NOBW
      IF(BETA(I,N,K).GT.0.0) BETA(I,N,K)=0.0
   82 CONTINUE
   18 WRITE(6,27)(BETA(I,J,K),J=1,NOBW)
    1 CONTINUE
C
C. READ TOTAL WATER REQUIRED(MT**3/SEC) DURING THE PLANNING
PERIOD
C
      READ(5,30) QTOT
      WRITE(6,31)QTOT
   30 FORMAT(F10.0)
   31 FORMAT(F10.3)
C
C. READ IN INDICES OF DRAWDOWN OBSERVATION WELLS
C
      READ(5,66) (IIO(K),JJO(K),KKO(K),K=1,NOBW)
      WRITE(6,66) (IIO(K),JJO(K),KKO(K),K=1,NOBW)
   66 FORMAT(24I3)
C
C. READ IN UPPER BOUNDS OF PUMPAGE FOR EACH PUMPING/INJECTION
WELL
C
      READ(5,99) (UPBQ(K),K=1,NTW)
      WRITE(6,98) (UPBQ(K),K=1,NTW)
   99 FORMAT(10F5.0)
   98 FORMAT(10F5.2)
C
C. READ IN LOWER BOUND OF PUMPAGE FOR EACH TIME STEP FOR EACH
WELL
C
      DO 55 IT=1,NTS
      READ(5,43) (QLB(K,IT),K=1,NTW)
      WRITE(6,433) (QLB(K,IT),K=1,NTW)
   43 FORMAT(8F8.0)
  433 FORMAT(8F8.3)
   55 CONTINUE
C
C. READ IN LOWER BOUND OF PUMPAGE FOR EACH TIME STEP FOR THE
AREA
C
      READ(5,40) (QMIN(IT),IT=1,NTS)
      WRITE(6,41) (QMIN(IT),IT=1,NTS)
   40 FORMAT(10F8.0)
   41 FORMAT(7F8.3)
C
C. READ IN UPPER BOUNDS TO DRAWDOWNS(MT) AT EACH DESIRED
LOCATION
C
      READ(5,45) (SMAX(K),K=1,NOBW)
      WRITE(6,451) (SMAX(K),K=1,NOBW)
   45 FORMAT(8F8.0)
  451 FORMAT(8F8.2)
```

```
C.
C. READ UNMANAGED HEADS AT DESIRED LOCATIONS AT EACH TIME
C.
      DO 88 IT=1,NTS
      READ(5,27) (HI(K,IT),K=1,NOBW)
C     WRITE(6,453) (HI(K,IT),K=1,NOBW)
C 452 FORMAT(6F10.0)
  453 FORMAT(6F10.2)
   88 CONTINUE
C
C. WRITE SECTION
C
      WRITE(6,33) NPW,NOBW
   33 FORMAT(//' NUMBER OF PUMPING WELLS =',I3,/' NUMBER OF
     1OBSERVATION WELLS =',I3/)
      WRITE(6,39) STIME
   39 FORMAT('   SCALING   TIME   FACTOR   FOR   BETAS   =',F12.1,'
SECONDS')
      WRITE(6,300) QTOT
  300 FORMAT('  TOTAL  WATER  DEMAND  FOR  THE  PLANNING  PERIOD
=',F10.4)
      WRITE(6,207) (QMIN(IT),IT=1,NTS)
  207 FORMAT(5X,'LOWER LIMIT OF PUMPAGE FOR AREA DURING EACH
     1TIME STEP',/10F8.4)
      WRITE(6,208) (IIO(K),JJO(K),K=1,NOBW)
  208 FORMAT(5X,'INDICES OF DRAWDOWN OBSERVATION WELLS',/,
     124I3)
      WRITE(6,210) (K,SMAX(K),K=1,NOBW)
  210 FORMAT(//,' MAXIMUM DRAWDOWN OF OBSERVATIN WELLS',//5X,
     1'OBSERVATION WELL',5X,' DRAWDOWN (MT)'/(5X,I4,15X,F7.2))
C  28 FORMAT( //' BETA(',I2,',J,',I2,')'/(8E15.5))
   27 FORMAT(5E15.5)
      WRITE(6,225) (IT,IT=1,NTS)
  225 FORMAT('1',2X,'MIN REQUIRED PUMP FOR EACH TIME STEP FOR
     1EACH PUMP WELL',//,2X,'WELL',10I7,/)
      DO 400 K=1,NPW
  400 WRITE(6,301) K,(QLB(K,IT),IT=1,NTS)
  301 FORMAT(I5,3X,10F7.3)
      CALL MATGEN
      STOP
      END
      SUBROUTINE MATGEN
C
C  *** THIS SUBROUTINE GENERATES THE LP MATRIX IN MPS FORMAT***
C
      COMMON /C01/ BETA(60,120,20)
      COMMON /C02/ NPW,NOBW,NTS,NPAIR,NIW,NTW
      COMMON /C03/ UPBQ(60),SMAX(120),QMIN(60),QTOT
      COMMON /C04/ ITITLE(2),HI(120,20)
      COMMON /C05/ QLB(60,20)
C
C.GENERATE THE SPECS FILE
C ----------------------
      WRITE(9,3500) ITITLE
 3500 FORMAT('BEGIN',1X,2A4)
      WRITE(9,3001)
 3001 FORMAT(3X,'MINIMIZE')
```

```
      WRITE(9,3002)
 3002 FORMAT(3X,'OBJECTIVE MINQIW')
      WRITE(9,3003)
 3003 FORMAT(3X,'ROWS',6X,'3000')
      WRITE(9,3004)
 3004 FORMAT(3X,'COLUMNS',3X,'6000')
      WRITE(9,3005)
 3005 FORMAT(3X,'ELEMENTS',3X,'1500000')
      WRITE(9,3105)
 3105 FORMAT(3X,'MPS FILE',3X,'10')
      WRITE(9,3006)
 3006 FORMAT(3X,'SCALE YES')
      WRITE(9,3007) ITITLE
 3007 FORMAT('END',1X,2A4)
C
C.GENERATE THE MPS FILE
C ---------------------
      WRITE(8,2008) ITITLE
 2008 FORMAT('NAME',T15,2A4)
      WRITE(8,2009)
 2009 FORMAT('ROWS')
C
C.SET UP ROW NAMES
C ----------------
C.   1) TOTAL PUMPAGE FOR AREA FOR ALL TIME STEPS
C
      WRITE(8,2010)
 2010 FORMAT(1X,'G  TOTQ')
C
C.   2) TOTAL DEMAND FOR EACH TIME STEP
C
      DO 100 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2011) IT1,IT2
 2011 FORMAT(1X,'G  TQ',2I1)
  100 CONTINUE
C
C.   3) DRAWDOWN FOR EACH OBSERVATION WELL & EACH TIME STEP
C
      DO 105 IW=1,NOBW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      DO 105 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2012) IW1,IW2,IW3,IT1,IT2
 2012 FORMAT(1X,'E  D',5I1)
  105 CONTINUE
C.
C.   4)  GRADIENT CONTROL CONSTRAINTS, C
C.
      DO 115 IW=1,NPAIR
      IW1=IW/10
      IW2=IW-IW1*10
```

```
      DO 115 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2013) IW1,IW2,IT1,IT2
 2013 FORMAT(1X,'G  C',4I1)
  115 CONTINUE
C
C.   5) TOTAL INJECTION < TOTAL PUMPAGE FOR EACH TIME STEP
C

      DO 280 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2031) IT1,IT2
 2031 FORMAT(1X,'G  PI',2I1)
  280 CONTINUE
C
C.   6) OBJECTIVE FUNCTION NAME
C
      WRITE(8,2015)
 2015 FORMAT(1X,'N  MINQIW')
C
C.SET UP COEFFICIENTS OF COLUMNS
C ------------------------------
C
      WRITE(8,2017)
 2017 FORMAT('COLUMNS')
C
C. ENTER COEFFICIENTS OF PUMPING RATES FOR DEMAND WELLS:
C
      DO 145 IW=1,NPW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      DO 145 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C                    1) TOTQ EQUATION
C
      WRITE(8,2018) IW1,IW2,IW3,IT1,IT2
 2018 FORMAT('    Q',5I1,T15,'TOTQ',T25,'0.000001E+06')
C
C                    2) TQ(T) EQUATION
C
      WRITE(8,2019) IW1,IW2,IW3,IT1,IT2,IT1,IT2
 2019 FORMAT('    Q',5I1,T15,'TQ',2I1,T25,'0.000001E+06')
C
C                    3) PI(T) EQUATION
C
      WRITE(8,2059) IW1,IW2,IW3,IT1,IT2,IT1,IT2
 2059 FORMAT('    Q',5I1,T15,'PI',2I1,T25,'0.000001E+06')
C
C                    4) DRAWDOWN D(W,T) EQUATIONS
C
      JJ=IW
```

```
      DO 140 II=1,NOBW
      IWW1=II/100
      IWW4=II-IWW1*100
      IWW2=IWW4/10
      IWW3=IWW4-IWW2*10
      IS=IT
      KK=0
      DO 135 I=IS,NTS
      ITT1=I/10
      ITT2=I-ITT1*10
      KK=KK+1
      TAIJ=-BETA(JJ,II,KK)
      WRITE(8,2020)IW1,IW2,IW3,IT1,IT2,IWW1,IWW2,IWW3,ITT1,ITT2,
      TAIJ
 2020 FORMAT('    Q',5I1,T15,'D',5I1,T25,E12.6)
  135 CONTINUE
  140 CONTINUE
C
C                    5) OBJECTIVE FUNCTION COEFFICIENTS
C
      IF(IW.LE.NPW) GO TO 145
      WRITE(8,4020) IW1,IW2,IW3,IT1,IT2
 4020 FORMAT('    Q',5I1,T15,'MINQIW',T25,'0.000001E+06')
  145 CONTINUE
C
C.      ENTER COEFFICIENTS OF PUMPING RATES FOR GRADIENT WELLS
C
      DO 445 IW=1,NIW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      DO 445 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C                     1) PI(T) EQUATION
C
      WRITE(8,2061) IW1,IW2,IW3,IT1,IT2,IT1,IT2
 2061 FORMAT('    P',5I1,T15,'PI',2I1,T25,'0.000001E+06')
C
C                     2) DRAWDOWN D(W,T) EQUATIONS
C
      JJ=NPW+IW
      DO 440 II=1,NOBW
      IWW1=II/100
      IWW4=II-IWW1*100
      IWW2=IWW4/10
      IWW3=IWW4-IWW2*10
      IS=IT
      KK=0
      DO 435 I=IS,NTS
      ITT1=I/10
      ITT2=I-ITT1*10
      KK=KK+1
```

```
      TAIJ=BETA(JJ,II,KK)
      WRITE(8,7037)IW1,IW2,IW3,IT1,IT2,IWW1,IWW2,IWW3,ITT1,ITT2,
      TAIJ
 7037 FORMAT('    P',5I1,T15,'D',5I1,T25,E12.6)
  435 CONTINUE
  440 CONTINUE
C
C                    3) OBJECTIVE FUNCTION COEFFICIENTS
C
      WRITE(8,4120) IW1,IW2,IW3,IT1,IT2
 4120 FORMAT('    P',5I1,T15,'MINQIW',T25,'0.000001E+06')
  445 CONTINUE
C
C.      ENTER COEFFICIENTS OF INJECTION RATES FOR GRADIENT WELLS
C
      DO 545 IW=1,NIW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      DO 545 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                   1) PI(T) EQUATION
C
      WRITE(8,2071) IW1,IW2,IW3,IT1,IT2,IT1,IT2
 2071 FORMAT('    I',5I1,T15,'PI',2I1,T25,'-0.00001E+05')
C
C.                   2) DRAWDOWN D(W,T) EQUATIONS
C
      JJ=NPW+IW
      DO 540 II=1,NOBW
      IWW1=II/100
      IWW4=II-IWW1*100
      IWW2=IWW4/10
      IWW3=IWW4-IWW2*10
      IS=IT
      KK=0
      DO 535 I=IS,NTS
      ITT1=I/10
      ITT2=I-ITT1*10
      KK=KK+1
      TAIJ=-BETA(JJ,II,KK)
      WRITE(8,2120)IW1,IW2,IW3,IT1,IT2,IWW1,IWW2,IWW3,ITT1,ITT2,
      TAIJ
 2120 FORMAT('    I',5I1,T15,'D',5I1,T25,E12.6)
  535 CONTINUE
  540 CONTINUE
C
C.                  3) OBJECTIVE FUNCTION COEFFICIENTS
C
      WRITE(8,4021) IW1,IW2,IW3,IT1,IT2
 4021 FORMAT('    I',5I1,T15,'MINQIW',T25,'0.000001E+06')
  545 CONTINUE
C
C. ENTER COEFFICIENTS OF S(W,T):
```

```
C
      DO 200 IW=1,NTW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      DO 200 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1) DRAWDOWN D(W,T) EQUATION
C
      WRITE(8,2050) IW1,IW2,IW3,IT1,IT2,IW1,IW2,IW3,IT1,IT2
 2050 FORMAT('    S',5I1,T15,'D',5I1,T25,'0.000001E+06')
  200 CONTINUE
      NSG=NTW+1
      KPAIR=2
      KK=1
      IC=1
C
C. ENTER COEFFICIENTS OF S(W,T) IN OTHER EQUATIONS
C
      TA=1.
      DO 500 IW=NSG,NOBW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      TB=-TA
      IC1=IC/10
      IC2=IC-IC1*10
      IF(KK.NE.KPAIR) GO TO 75
      KK=0
      IC=IC+1
   75 KK=KK+1
      DO 501 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1)DRAWDOWN EQUATIONS
C
      WRITE(8,2060) IW1,IW2,IW3,IT1,IT2,IW1,IW2,IW3,IT1,IT2
 2060 FORMAT('    S',5I1,T15,'D',5I1,T25,'0.000001E+06')
C
C.                    2) GRADIENT CONTROL EQUATIONS
C
      WRITE(8,2051) IW1,IW2,IW3,IT1,IT2,IC1,IC2,IT1,IT2,TB
 2051 FORMAT('    S',5I1,T15,'C',4I1,T25,E12.6)
  501 CONTINUE
      TA=-TA
  500 CONTINUE
C
C. ENTER COEFFICIENTS OF U(W,T):
C
      DO 220 IW=1,NTW
      IW1=IW/100
      IW4=IW-IW1*100
```

```
      IW2=IW4/10
      IW3=IW4-IW2*10
      DO 220 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1) DRAWDOWN D(W,T) EQUATION
C
      WRITE(8,2250) IW1,IW2,IW3,IT1,IT2,IW1,IW2,IW3,IT1,IT2
 2250 FORMAT('    U',5I1,T15,'D',5I1,T25,'-0.00001E+05')
  220 CONTINUE
      NSG=NTW+1
      KPAIR=2
      KK=1
      IC=1
C
C. ENTER COEFFICIENTS OF U(W,T) IN OTHER EQUATIONS
C
      TC=-1.
      DO 510 IW=NSG,NOBW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      TD=-TC
      IC1=IC/10
      IC2=IC-IC1*10
      IF(KK.NE.KPAIR) GO TO 76
      KK=0
      IC=IC+1
   76 KK=KK+1
      DO 601 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
C
C.                    1)DRAWDOWN EQUATIONS
C
      WRITE(8,3061) IW1,IW2,IW3,IT1,IT2,IW1,IW2,IW3,IT1,IT2
 3061 FORMAT('    U',5I1,T15,'D',5I1,T25,'-0.00001E+05')
C
C.                    2)GRADIENT CONTROL EQUATIONS
C
      WRITE(8,3071) IW1,IW2,IW3,IT1,IT2,IC1,IC2,IT1,IT2,TD
 3071 FORMAT('    U',5I1,T15,'C',4I1,T25,E12.6)
  601 CONTINUE
      TC=-TC
  510 CONTINUE
C
C. SET UP RIGHT-HAND SIDE:
C ----------------------
      WRITE(8,2029)
 2029 FORMAT('RHS')
C
C.                    1) TOTQ EQUATION
C
      WRITE(8,2030) QTOT
 2030 FORMAT(T5,'RHS1',T15,'TOTQ',T25,F12.4)
```

```
C
C.                     2) TOTAL DEMAND FOR EACH TIME STEP
C
      DO 3000 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,7031) IT1,IT2,QMIN(IT)
 7031 FORMAT(T5,'RHS1',T15,'TQ',2I1,T25,E12.6)
 3000 CONTINUE
C
C. ENTER RHS OF GRADIENT CONTROL CONSTRAINTS
C
      JP=1
      DO 777 IC=1,NPAIR
      II1=NTW+JP
      II2=II1+1
      IC1=IC/10
      IC2=IC-IC1*10
      JP=JP+2
      DO 777 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      GRHS=HI(II2,IT)-HI(II1,IT)
      WRITE(8,778) IC1,IC2,IT1,IT2,GRHS
  778 FORMAT(T5,'RHS1',T15,'C',4I1,T25,E12.6)
  777 CONTINUE
C
C. ENTER RHS OF PI CONSTRAINTS SO THAT THEY ARE EQUAL TO DEMAND
C
      DO 3033 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      PIRHS=QMIN(IT)
      WRITE(8,7047) IT1,IT2,PIRHS
 7047 FORMAT(T5,'RHS1',T15,'PI',2I1,T25,E12.6)
 3033 CONTINUE
C
C. SET UP BOUNDS SECTION:
C  ---------------------
      WRITE(8,2034)
 2034 FORMAT('BOUNDS')
C
C.              1) LOWER & UPPER PUMPING LIMITS FOR DEMAND WELLS
C
      DO 175 IW=1,NPW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      DO 175 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,2038) IW1,IW2,IW3,IT1,IT2,QLB(IW,IT)
 2038 FORMAT(' LO BOUND ',T15,'Q',5I1,T25,E12.6)
      WRITE(8,2035) IW1,IW2,IW3,IT1,IT2,UPBQ(IW)
 2035 FORMAT(' UP BOUND ',T15,'Q',5I1,T25,E12.6)
  175 CONTINUE
```

```
      DO 278 IW=1,NIW
      IW1=IW/100
      IW4=IW-IW1*100
      IW2=IW4/10
      IW3=IW4-IW2*10
      IK=NPW+IW
      DO 278 IT=1,NTS
      IT1=IT/10
      IT2=IT-IT1*10
      WRITE(8,5035) IW1,IW2,IW3,IT1,IT2,UPBQ(IK)
 5035 FORMAT(' UP BOUND ',T15,'P',5I1,T25,E12.6)
      WRITE(8,5036) IW1,IW2,IW3,IT1,IT2,UPBQ(IK)
 5036 FORMAT(' UP BOUND ',T15,'I',5I1,T25,E12.6)
  278 CONTINUE
      WRITE(8,2036)
 2036 FORMAT('ENDATA')
      WRITE(6,2037)
 2037 FORMAT(5X,'**** MATRIX FOR LP IS GENERATED ON UNIT 8
****')
      RETURN
      END
```