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Analytical Modeling of Particle Tracking for Dynamic Pumping Conditions

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Abstract: Movement of fluid particles about historic subsurface releases and through well fields is often governed by dynamic subsurface water levels. Motivations for tracking the movement of fluid particles include tracking the fate of subsurface contaminants and resolving the fate of water stored in subsurface aquifers. Based on superposition of the Theis solution in both space and time, this research explores an analytical solution based on the Theis equation using dynamic pumping well data to resolve how fluid particles move around wells under dynamic pumping conditions. The results provide relatively uniform capture zones for a pumping well. Further, the results show that even under continuous pumping and injection conditions, groundwater will not flow far from the well. Accordingly, groundwater positions can be evaluated based on the research for dynamic pumping. Using the assumptions proposed by the Theis solution, the analytical solution developed in this study provides a simple method to evaluate particle movement in wells used to both store and recover water.

Keywords: particle tracking; dynamic pumping; analytical solution; well field

1. Introduction

Groundwater, which is distributed around the world, offers many advantages as a potable water source. The contamination of groundwater, however, is a widespread problem and requires solid techniques for its remediation [1–5]. Although many contaminants can be naturally attenuated in the subsurface via microorganism activity [6,7], residual chemicals can persist for a long period which poses substantial risks to natural groundwater resources, particularly public water supply well fields which are located at sites historically impacted by releases [8–11]. As such, consideration of capture zones in well fields under both pumping and injection stresses is an important issue.

To mitigate the threats of subsurface contaminants into fresh water resources around wells, efficient methods have been employed to track the flow of contaminants. Among these, particle tracking is commonly used to define the pathlines of solute particles under purely advective transport [12]. Particularly, particle-tracking schemes have been formally incorporated into solute transport models to account for the advective component of transport [13]. This basic idea follows the movement of infinitely small imaginary particles placed in a flow field using either analytical or numerical methods [14]. Particle tracking has been widely used in numerical modeling of groundwater flow to track contaminant paths. For example, [15] described the information on the regional groundwater flow field as "inferred from particle pathlines". Authors in [10] used a backward tracking method to delineate groundwater protection zones with an uncertainty analysis, applying a Monte Carlo approach coupled with the use of geographyical information systems. Authors in [1] presented the use of different global optimization (GO) algorithms to determine the optimized combination of pumping rates and well locations for the removal of a contaminant plume using particle tracking. Two modeling codes, MODFLOW and MODPATH [16], are commonly used for groundwater flow and particle tracking. Authors in [17] also used particle tracking to define flow paths of the recharge in some aquifers in Ghana, and the particle tracking simulation identified travel times in specific years from recharge areas to discharge areas along the flow paths. The conventional approach to groundwater protection is based on the concept of the wellhead protection area (WHPA) [18]. A wellhead protection area, as defined by U.S. EPA, is "the surface and subsurface area surrounding a water well or a well field, supplying a public water system, through which contaminants are reasonably likely to move toward and reach such water well or well field" [19]. A WHPA may comprise all or part of the capture zone from which the well draws its water [18].

To our knowledge, previous studies have not reported using analytical models to track particles under dynamic pumping conditions. As such, the objective of this study is to investigate whether the analytical solution is able to capture dynamic aspects of groundwater flow for complex water surfaces with dynamic water levels, e.g., pumping conditions. By making assumptions proposed by [20], an analytical model was developed from the Theis equation [20,21] that calculates head under dynamic pumping and injection conditions to evaluate particle tracking. The analytical solution is used to resolve the hydraulic gradient through a point of interest at a specified time, and incremental time steps are used to resolve particle flow path lines. Consideration is given to the prediction of flow under the influence of pumping and injection conditions.

2. Study Site and Dataset

2.1. Description of the Study Site

The study site was located in the town of Castle Rock, Colorado, where the Denver Basin groundwater is the primary water source [22,23]. The Denver Basin aquifer system is a group of confined, deep-bedrock sandstones located east of the Colorado Front Range. This field site is situated along the western flank of the Denver Basin aquifer system and is one of many towns included in the Front Range urban corridor [22]. There are four main well fields in Castle Rock. Data from the Meadows Pumping Center were used for analysis in this study. Well locations of the Meadows Pumping Center are shown in Figure 1. In this study, several assumptions of the aquifer and flow conditions were made. The aquifer of the Meadows Pumping Center was assumed to be of infinitely areal extent and homogeneous, isotropic, and of uniform thickness at 32.8 ft [22]. Transmissivity of the aquifer in the Meadows Pumping Center is 535 ft^2/day, storativity is 0.00005, and porosity was assumed to be 0.25 [22]. The wells in the center were assumed to be fully penetrating, and flow to the wells was horizontal. Further, groundwater was assumed to be released instantaneously from storage with decline of hydraulic head, and the diameters of pumping wells in Meadows Pumping Center were small enough that storage in the well could be neglected. These assumptions of the aquifer and groundwater flow conditions also led calculations of the drawdowns in the wells to follow the Theis solution described in Section 3.

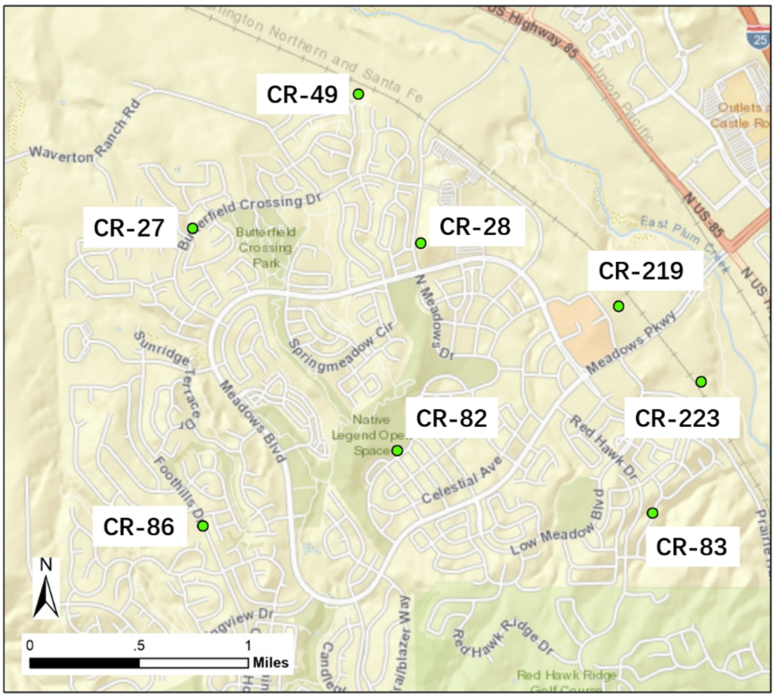
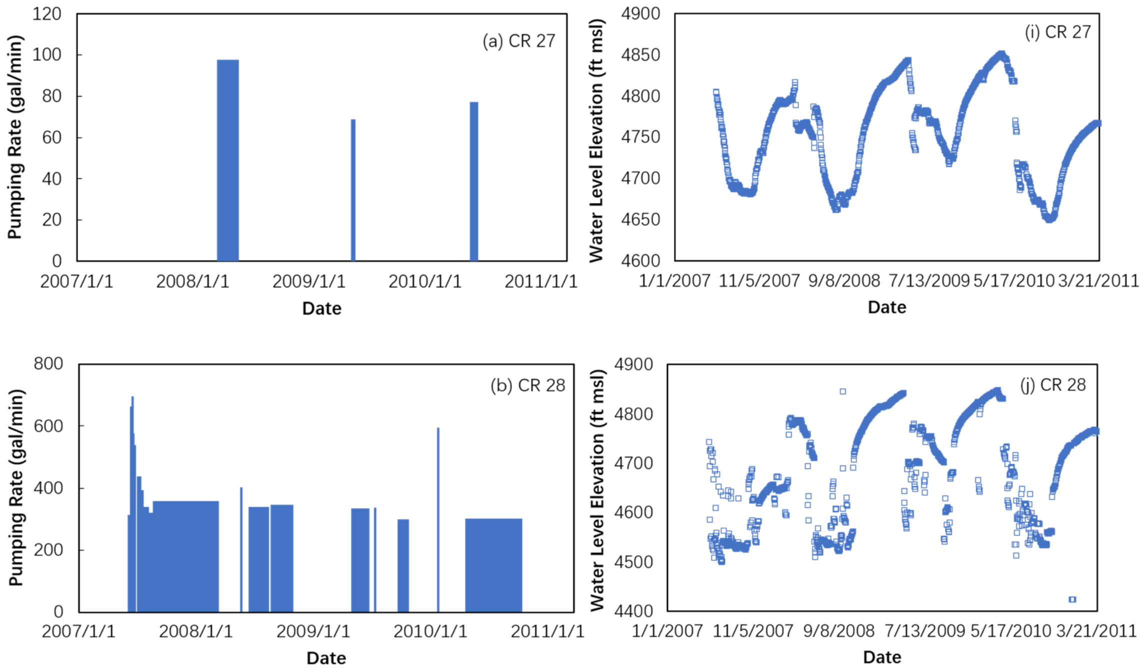


Figure 1. Well locations at the Meadows Pumping Center in Castle Rock, CO, USA.

2.2. Pumping and Water Level Data

There are eight wells operated at the Meadows Pumping Center [24]. Pumps in the eight wells cycled on and off from 2007 to 2011, and pumping rates are shown in Figure 2. Correspondingly, water levels in these eight wells continuously changed over this period (Figure 2). Daily frequency was used for the collections of pumping rates and water level data.



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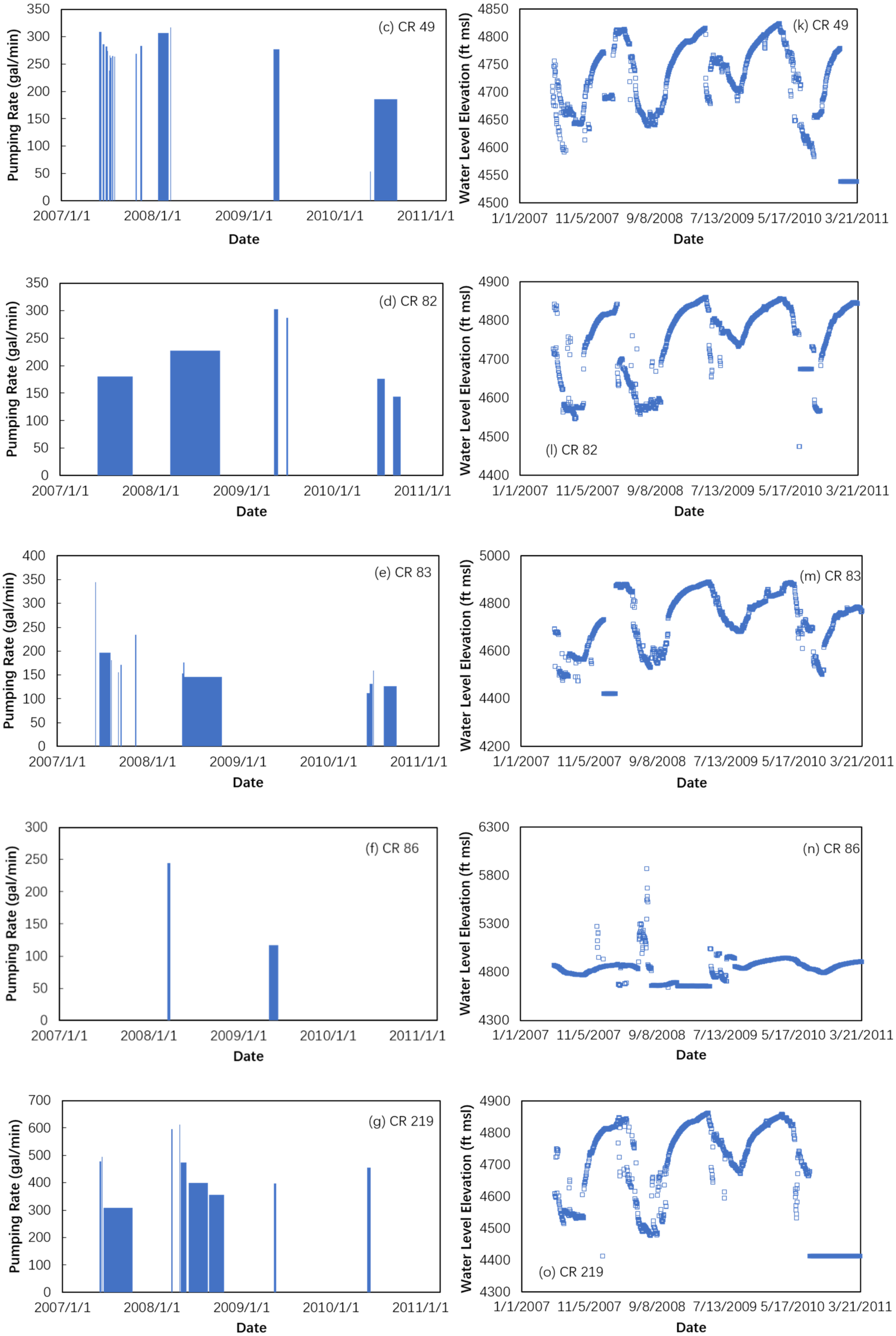

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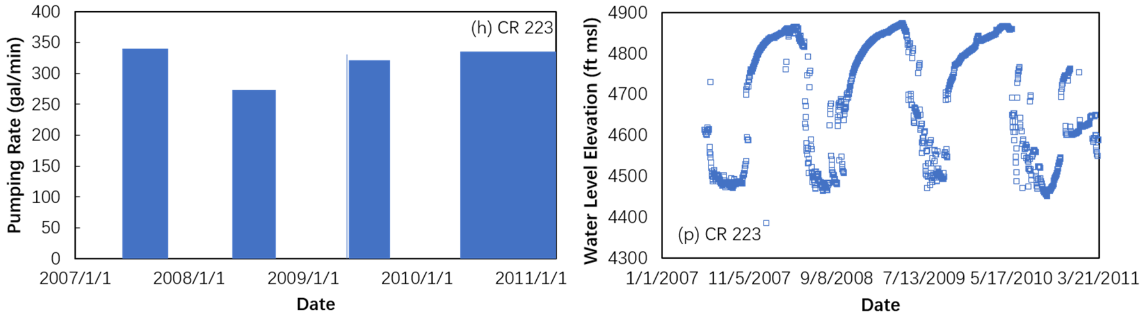


Figure 2. Pumping rates (**a**–**h**) and water levels (**i**–**p**) in eight wells at the Meadows Pumping Center, CO.

Owing to increased demand in groundwater and increased drawdowns, technologies that use recharge options, such as aquifer storage recovery (ASR), are used to optimize available water resources and reduce adverse effects of pumping [25]. Understanding the movement of injected water can help increase recovery efficiency, described as the percentage of water that can be recovered after injection [26].

Subsequently, in this study particle tracking under dynamic pumping and injection conditions were both considered. The injection process can be treated as the inverse process of pumping; therefore, the injection rate in the well field was set as the negative pumping rate. Specifically, particle tracking under continuous pumping and injection conditions were studied over 130 days and 6000 days, respectively. The reason for the longer period used for injection conditions is because a clear flow path of particle tracking can be observed. In this study, particle movement around well 82 was evaluated. The pumping and injection rates of well 82 correspond to the periods shown in Figure 3. Figure 3a shows a period of 130 days. The pumping rate of 244 gal/min was selected (Figure 2d), and −144 gal/min was assumed to be the injection rate. Figure 3b shows a period of 6000 days. The pumping rate of 244 gal/min was selected, and the injection rate was assumed to be −244 gal/min.

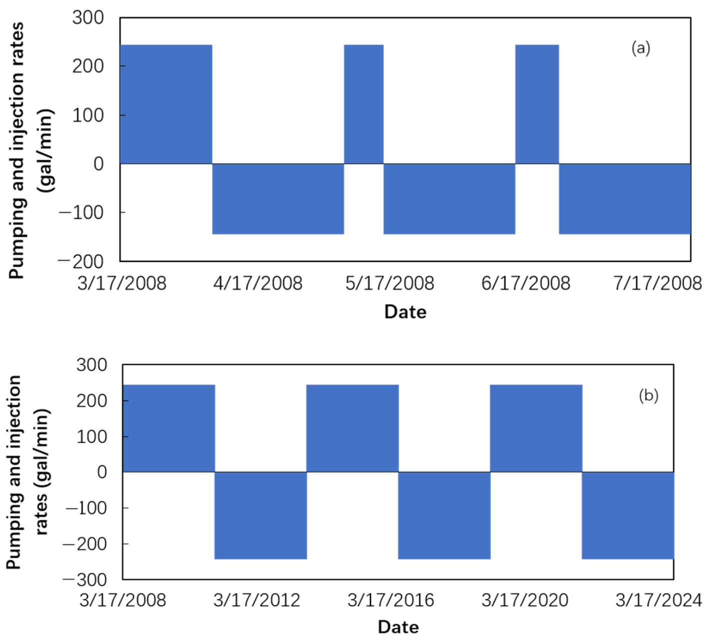


Figure 3. Pumping and injection rates employed for particle tracking over (**a**) 130 days and (**b**) 6000 days under continuous pumping and injection conditions at the Meadows Pumping Center, CO, USA.

3. Methods

Analytical methods are useful tools that can be applied to many groundwater flow problems, including estimation of travel time-related capture areas of wells in hydrogeologic settings with predominantly two-dimensional flow regimes [19]. Theis superposition model under these assumptions can successfully predict drawdown produced by multiple wells in well fields that are cycled on and off [20,21]. Dynamic water-level data are obtained through time with time-variant flow rates using the Theis superposition model. Data in [24] provide over three years of hourly water levels and pumping rates from operational well fields in Castle Rock, CO, USA. Further, [24] inputs well locations, pumping times associated with flow rates, as well as variables including transmissivity, storativity, natural slope of the potentiometric surface, and individual well loss constants into the Theis superposition model to calculate the drawdowns for all of its operational wells for more than three years. The Theis equation is [20,21]

$$s(r,t) = \frac{Q}{4\pi T}W(u) \tag{1}$$

where s is drawdown (L) at a particular radial distance r from the pumped well and time t since the start of pumping; Q is pumping rate (L^3T^{-1}); T is transmissivity (L^2T^{-1}); $W(u)$ is the well function that can be expressed as the infinite series [20,21]:

$$W(u) = -0.577216 - lnu + u - \frac{u^2}{2\times 2!} + \frac{u^3}{3\times 3!} - \frac{u^4}{4\times 4!} + \dots \tag{2}$$

with u being defined as

$$u = \frac{r^2 S}{4Tt} \tag{3}$$

where S is the storativity of the aquifer.

In a multiple well system, aquifer drawdown is influenced by more than one pumping well. Applying superposition of the Theis equation, the drawdown at any point in the aquifer can be calculated as the sum of the drawdown created by each well, individually. For a well field with n wells, associated pumping rates of $Q_1, Q_2, \dots, Q_n$, and radial distance from each well $r_1, r_2, \dots, r_n$, the following equation is used [20,21]:

$$s = \frac{Q_1}{4\pi T}W(u_1) + \frac{Q_2}{4\pi T}W(u_2) + \dots + \frac{Q_n}{4\pi T}W(u_n) \tag{4}$$

$$u_i = \frac{r_i^2}{4Tt_i} i = 1,2,\dots,n \tag{5}$$

with t_i defined as time from the start of pumping for wells with Q_i. Based on the Theis superposition model [20,21], this research developed a new analytical model to track particles under dynamic pumping conditions.

Following [20,21], the dynamic water head values are resolved as a function of position and time using superposition of the Theis solution in time and space for multiple wells with transient pumping. Inclusive to the methods of [20,21], we considered a regionally sloping potentiometric surface. Authors in [27] present additional developments for temporal and spatial superposition of the Theis solution for analysis of water levels in well fields.

A regression is performed to obtain a solution for the potentiometric surface (h, (L)) [28]:

$$h(x,y)_i = A_i x + B_i y + C \tag{6}$$

where x and y are positions of interest, A is the gradient of head in the x direction (dimensionless), B is the gradient of head in the y direction (dimensionless), C is a constant defined as the elevation of the water table at (0, 0) (L), and i is the time interval.

Under dynamic pumping conditions, head can be calculated by employing the static water surface elevations (h, (L)) minus the drawdown at any time [24]:

$$h(x, y, t)_i = A_i x + B_i y + C - \sum_{j=1}^{n} \sum_{i=1}^{m} s(x, y, t)_{ij} \quad (7)$$

and

$$t = t_{initial} + i\Delta t \quad (8)$$

where m is the total number of time steps, i is the number of time step, and j is the number of wells. $t_{initial}$ is the initial time when particles start to move (T); s_{ij} is the drawdown at time step i in the well j (L).

Applying this solution to the finite difference method, the hydraulic gradient is the difference of hydraulic head at two points adjacent to each other at any time divided by the distance between these two points. Hydraulic gradients in the x and y directions are used to drive particles based on hydraulic conductivity values. The equations are as follows:

$$A_i = \frac{h(x-1, y, t)_i - h(x+1, y, t)_i}{2} \quad (9)$$

$$B_i = \frac{h(x, y-1, t)_i - h(x, y+1, t)_i}{2} \quad (10)$$

The use of points 2 regarding the position of interest is based on a desire to accurately capture the local gradient, while not being close enough to the point of interest to introduce errors into the local gradient associated with computational accuracy of the method employed for estimating values of well functions [24].

According to Darcy's law and employing a succession of steady states, as with the field data approach, the initial positions of particle moving when time started are

$$x_{i=0} = x_{initial}, \text{ and } y_{i=0} = y_{initial} \quad (11)$$

When taking a particle forward in time:

$$x_{i+1} = x_i + \Delta x_i, \text{ and } y_{i+1} = y_i + \Delta y_i \quad (12)$$

where

$$\Delta x_i = \frac{-T}{b\varphi} A_i \Delta t_i, \text{ and } \Delta y_i = \frac{-T}{b\varphi} B_i \Delta t_i \quad (13)$$

where φ is effective porosity (dimensionless), and b is aquifer thickness (L).

Based on the assumptions of the aquifer and groundwater flow conditions made in Section 2, the pumping and injection rates described in Figure 3 were used in the analytical solution to track particles under dynamic pumping and injection conditions over different periods.

4. Results

The analytical solution used in this research was designed to obtain the time-dependent capture zone by placing particles around pumping wells, moving the particles backward from wells into the pumping field for injection conditions, and moving the particles forward from the pumping field into wells for pumping conditions, followed by connecting the particle positions at any given time with line segments. This solution captures the movement of subsurface fluid particles in pumping fields with dynamic water levels. Movement of particles was evaluated by (1) backward tracking of particles from the pumping field into the production wells, (2) forward tracking of particles from the injection wells into the pumping field, and (3) continuous pumping and injection conditions.

For pumping conditions, particle tracking was studied by backward methods. Initially, particles were tracked by starting with eight particles around one well, moving the particles from the aquifer to the well in time, and connecting the particle positions with line segments over 21 days. For injection conditions, particle tracking was studied by forward methods where particles were tracked from the well to the aquifer over time. Figure 4a,b shows the flow paths of particles under pumping and injection conditions, respectively. The results indicated that if we know the current particle position, we can use particle tracking to determine where the particles were and even their location a few days prior under pumping and injection conditions.

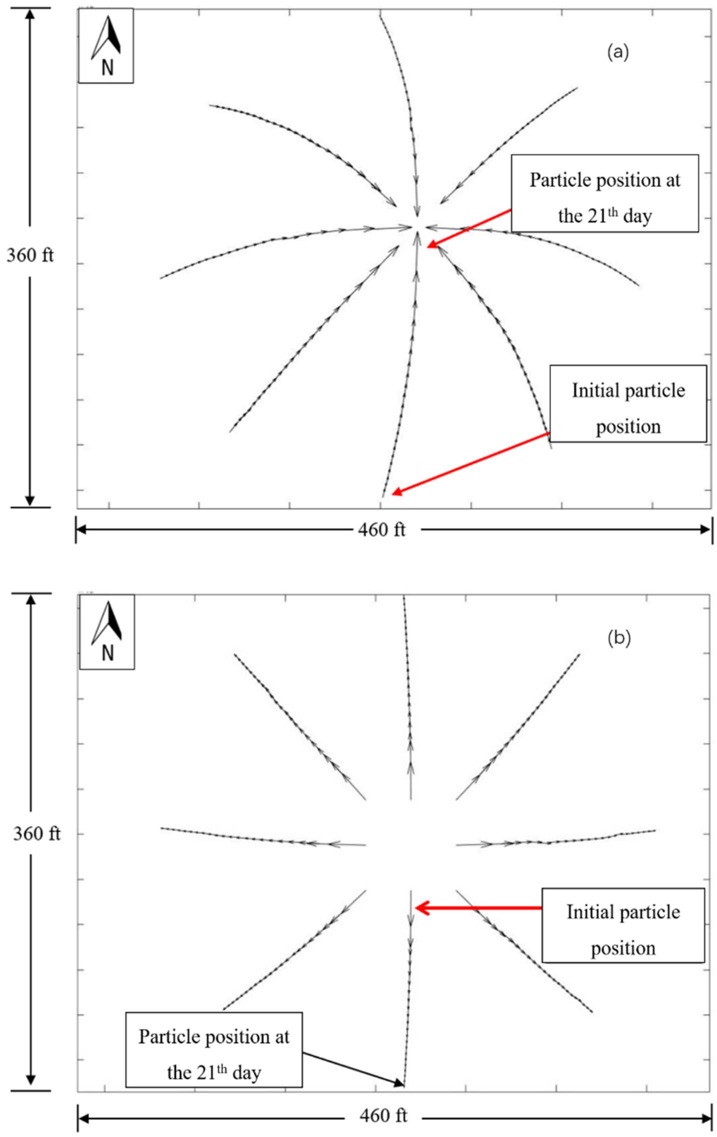


Figure 4. Movement of particles around one representative of eight wells for 21 days under (**a**) pumping and (**b**) injection conditions at the Meadows Pumping Center, CO, USA.

When pumping stops, water levels in the well and aquifer may rise toward pre-pumping levels. Due to pumps being continuously on and off, uninterrupted drawdowns and recoveries happened successively. Figure 5 shows how particles move under continuous pumping and injection conditions in a well over time. Associated pumping stress is shown in Figure 3a. In Figure 5, water was initially pumped from a well for 21 days (0–1 shown in the figure), and then the water was injected into the well for 30 days (1–2 shown in the figure). A similar process for the residual steps is shown in Figure 5. These pumping and injection processes were continued for a total of 130 days.

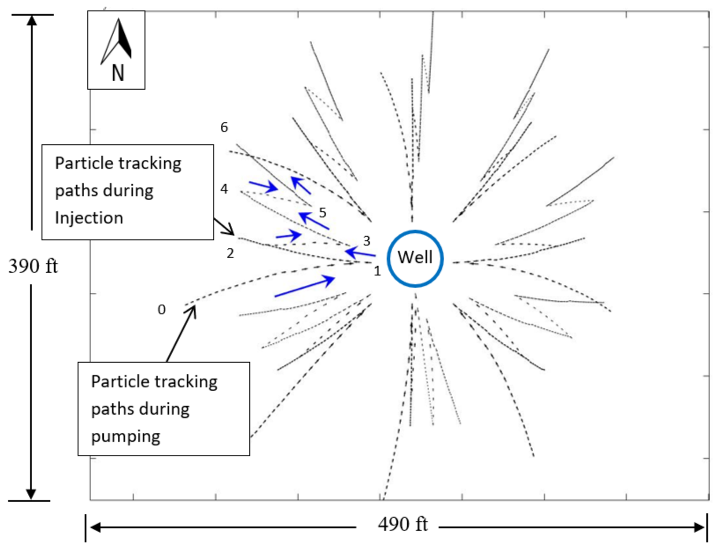
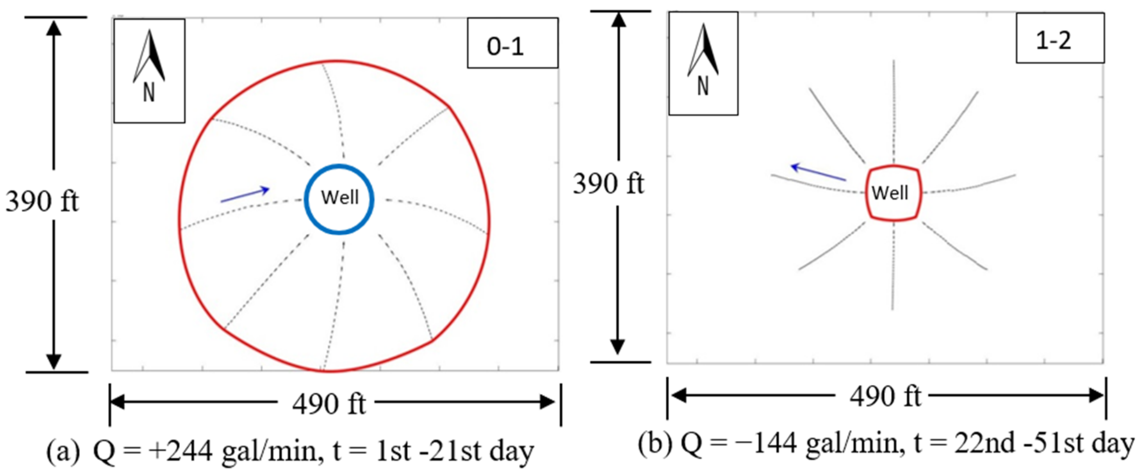


Figure 5. Movement of particles around one representative of eight wells for 130 days under continuous pumping and injection conditions at the Meadows Pumping Center, CO, USA. The blue arrows represent the particle flow directions in pumping and injection processes. The numbers are used to illustrate particle positions at the beginning or end of pumping and injection processes.

The movement of water under each pumping and injection process is shown in Figure 6. The red circle represents the water position under each pumping and injection process. When the pumps turn on and off, groundwater levels fall and rise continuously. The injection process drives rising water levels. Accordingly, particles flow towards the well when the pump is on and flow away when the water is injected. The injection curve is nearly an inverted image of the drawdown curve. The resulting inverted paths were less symmetric because the well in Figure 5 was in a well field influenced by seven other wells in the Meadows Pumping Center, although they were far away from each other (Figure 1); drawdown in this well was accordingly influenced by other drawdowns during the pumping process.



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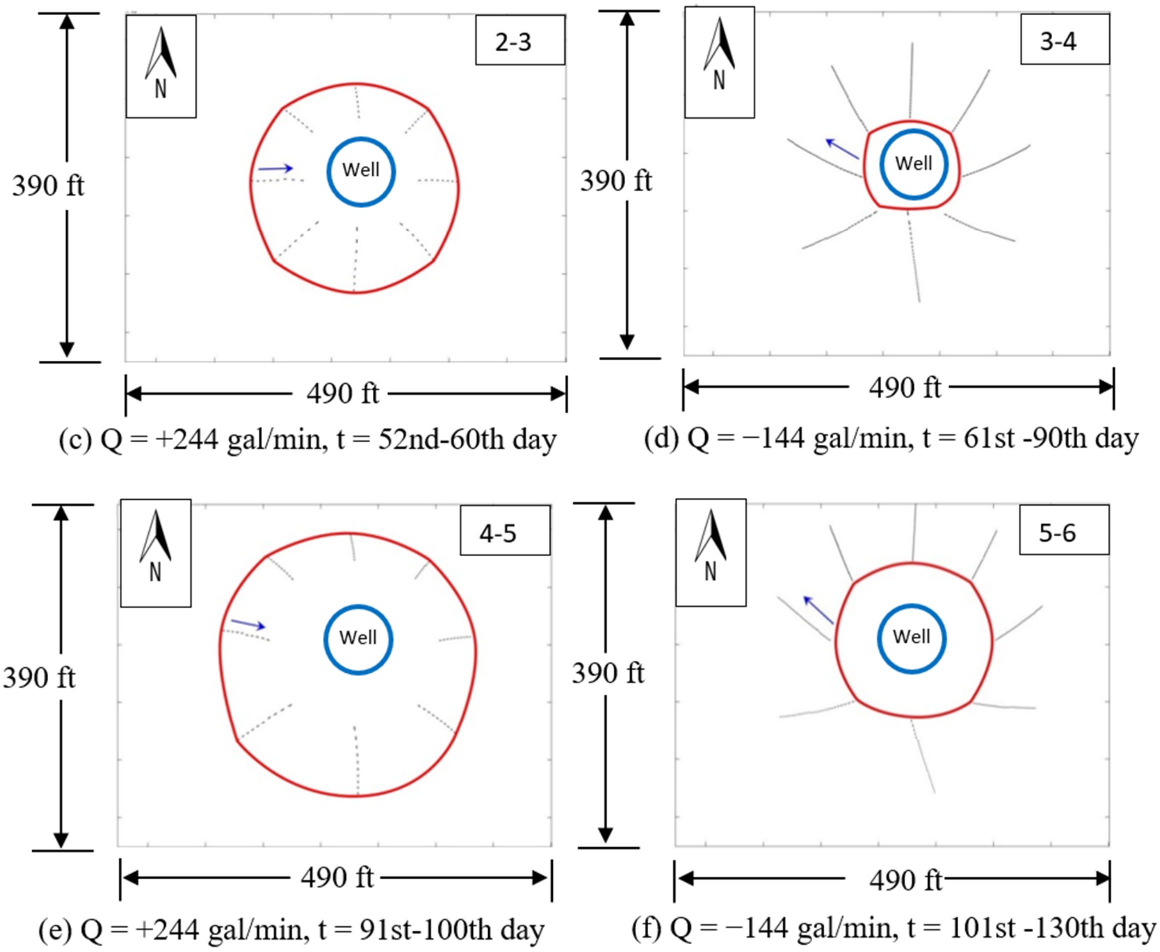


Figure 6. Water circles around a well for 130 days under pumping and injection conditions at the Meadows Pumping Center, CO, USA. (**a**,**c**,**e**) represent the pumping process during the periods of the 1st–21st day, 52nd–60th day, and 91st–100th day. (**b**,**d**,**f**) represent the injection process during the periods of the 22nd–51st day, 61st–90th day, and 101st–130th day.

5. Discussion

Particle tracking under continuous pumping and injection conditions was studied for a longer period of time in order to see if similar results could be obtained. Figure 7 shows the movement of water for 6000 days under continuous pumping and injection conditions. Uninterrupted drawdowns and recoveries also occurred successively because of continuous pumping and injection. The associated pumping stress is shown in Figure 3b. The movement of water under each pumping and injection process is shown in Figure 8. The red circle represents the water position under each pumping and injection process.

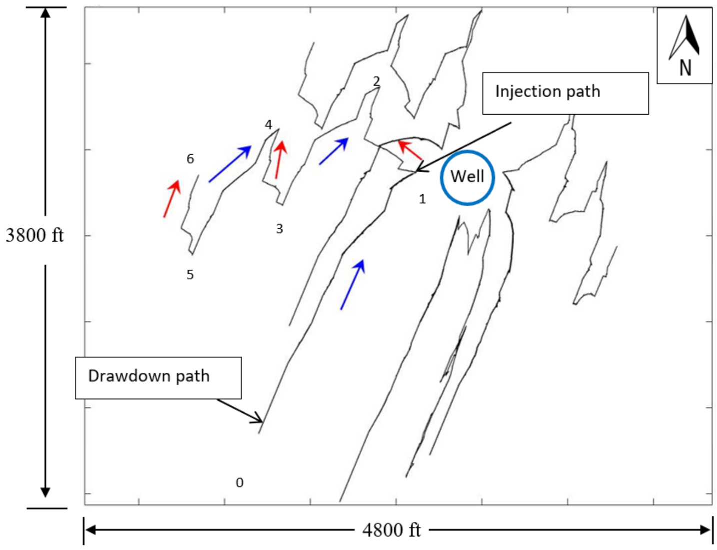
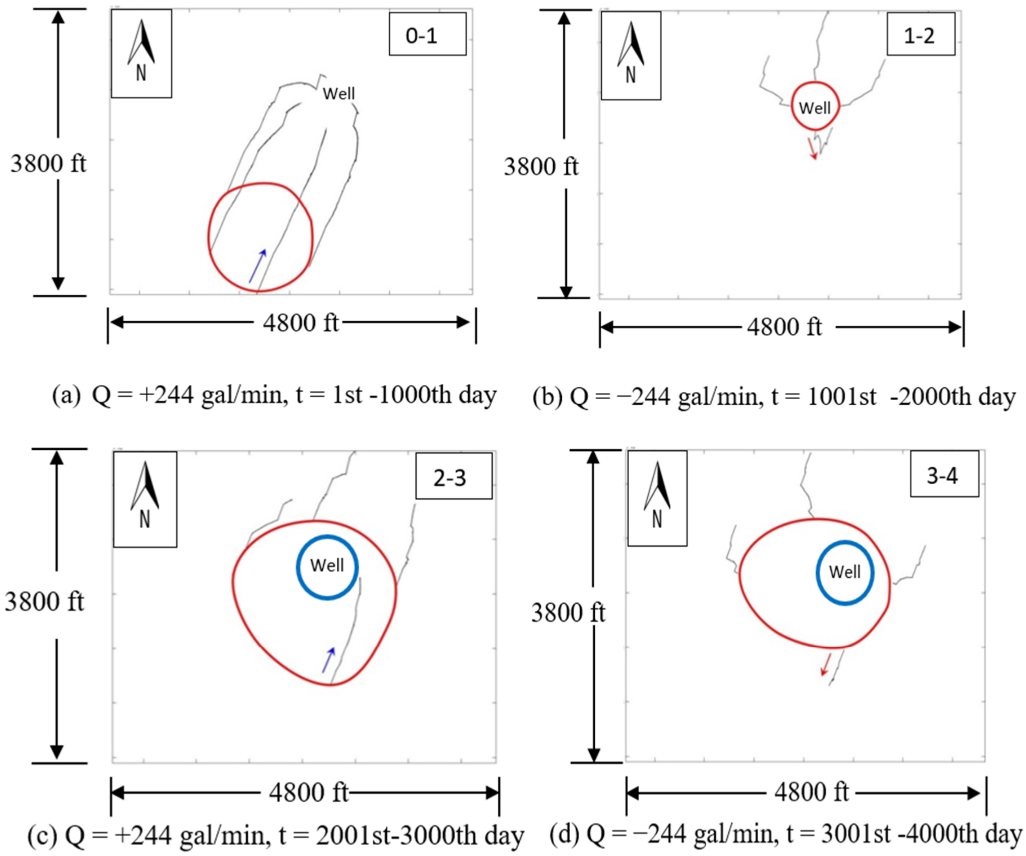


Figure 7. Movement of particles around one representative of eight wells for 6000 days under continuous pumping and injection conditions at the Meadows Pumping Center, CO, USA. The blue and red arrows represent the particle flow directions under pumping and injection processes, respectively. The numbers represent particle positions at the beginning or end of pumping and injection processes.



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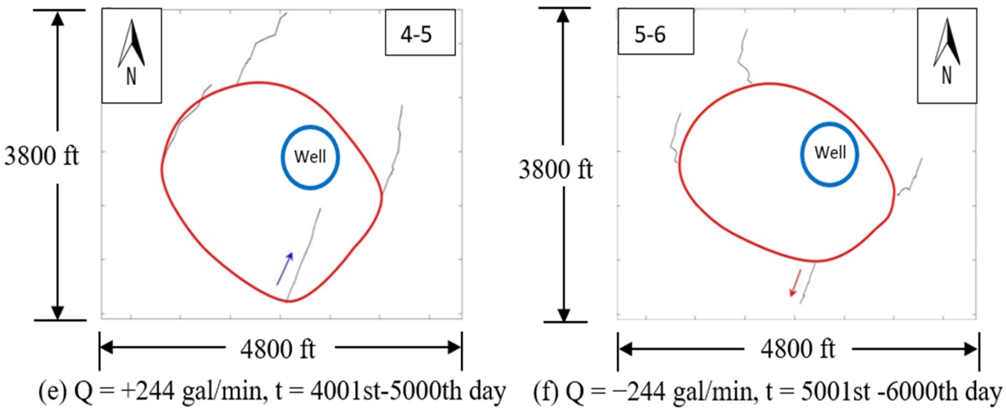

Figure 8. Water circles around a well for 6000 days under pumping and injection conditions at the Meadows Pumping Center, CO, USA. (**a**,**c**,**e**) represent the pumping process during the periods of the 1st–1000th day, 2001st–3000th day, and 4001st–5000th day. (**b**,**d**,**f**) represent the injection process during the periods of the 1001st–2000th day, 3001st–4000th day, and 5001st–6000th day.

For a longer period of time, i.e., 6000 days in this case, water did not flow far away from the well under continuous pumping and injection. For the first 1000 days (Figure 8a), water moved 861.12 ft from the aquifer to the well during pumping. In Figure 8b, water was injected into the aquifer and moved 183.1 ft back to the aquifer from the well. In the following processes (Figure 8c,d), water moved 513.81 ft from the aquifer to the well and 176.41 ft from the well back to the aquifer. Finally, water again moved 659.45 ft from the aquifer to the well and 180.84 ft from the well back to the aquifer (Figure 8d,f). Based on these results, the analytical method could provide the movement of particles under pumping conditions.

The aim of this study is to use dynamic water level data and an analytical solution developed from the Theis equation to track particles under dynamic pumping conditions. Therefore, the focus of this study is the analytical method. The settings of geologic parameters referred to literature on the study site, and several assumptions of the aquifer and flow conditions were made. These assumptions were used to testify the method. This method can be used with various assumptions; therefore, limitations exist for the method. For example, it is not applicable in heterogeneous and anisotropic conditions. Further, although several assumptions applicable to the Theis equation have been made, lab or field experiments can be conducted to verify results.

6. Conclusions

Groundwater in well fields has the potential to become contaminated by organic or inorganic compounds from releases. For field sites with dynamic pumping conditions, this research explored an analytical solution developed from the Theis superposition model [20,21] to solve particle tracking under dynamic pumping conditions with space and time. A well field was employed in this study to predict the movement of groundwater by tracking particles under dynamic pumping and injection conditions, relying on dynamic water-level data and the analytical solution.

The Theis superposition model [20,21] provided exact solutions for gradients about pumping wells under dynamic pumping conditions. Based on the Theis superposition model and the analytical solution, flow path lines of fluid particles under dynamic pumping and injection conditions at well fields were obtained. Under dynamic pumping conditions, the results of this study provided relatively uniform capture zones. The results showed that, although groundwater may flow away from the well to the aquifer during the pumping process, and flow toward the well from the aquifer during the injection process, positions of the groundwater may change following each process, but it does not flow far away from the well. Accordingly, groundwater positions can be evaluated based on the research for dynamic pumping. Under specific assumptions, the analytical solution developed in this study provides a clue or even a simple method to evaluate particle movement about well fields used to both store and recover water.

Limitations exist in this analytical method as it was developed by making several assumptions of the aquifer and flow conditions. For tracking particles in heterogeneous and anisotropic conditions, or if the aquifers are highly recharge affected (e.g., karst aquifers) under dynamic pumping conditions, this method may not be applicable. Further research may focus on developing simple analytical methods for tracking particles in complex aquifers, flow, and hydrologic conditions. Moreover, field experiments or numerical solutions need to be conducted to verify results derived from the analytical methods.

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