Simulating-optimizing coupled method for pumping well layout at a nitrate-polluted groundwater site

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Abstract. The unreasonable pumping scheme of the pump-treat technology can lead to high repair cost and poor performance in contaminated groundwater remediation. In order to improve the cost effectiveness of the technology, we took a heavily nitrate-polluted informal domestic waste landfill site in North China as an example, and optimized the pumping scheme using Visual MODFLOW software combined with genetic algorithm (GA) in MGO module. By designing the constant pumping rate scheme and phased pumping rate scheme, optimal layout of pumping wells were determined with the minimum total pumping capacity as the optimal target. The result showed that the two wells which located near the central axis and in the middle and lower reaches of the plume with a constant pumping rate of 13.2 m³/d and continuous pumping for 75 days was the optimal pumping solution in constant pumping rate scheme. While the pump schedule as \( Q_1 = 19.8 \text{ m}^3/\text{d}, Q_2 = 6.93 \text{ m}^3/\text{d}, t_1 = 25 \text{ d}, t_2 = 50 \text{ d} \) express the minimum total water output which was the optimal pumping scheme in phased pumping rate scheme. By comparing the two schemes, it was concluded that under the same governance days, the phased pumping scheme could save 15% of the total pump output compared with the constant pumping scheme.

1. Introduction

The shortage and degradation of drinking water sources are global hotspot issues of mutual interest. Groundwater pollution is difficult to manage and recovering the water quality may take years and sometimes more than a decade even the pollution source have been removed. The heavy time and economic costs of ground water remediation make it a huge challenge in the water resources field. The pump and treat technology refers to the process of pumping contaminated groundwater to the surface for purification treatment to reduce the groundwater pollutants [1-5]. The core of the technology is setting the well location and well number reasonably based on the hydrogeological condition of a contaminated site to form a hydraulic capture zone [6-8]. The pump and treat technology had been widely used since mid-1980s. The United States Environmental Protection Agency (EPA) and scholars began to pay close attention to the design of the system in the early 1990s [9-11]. Recently, more research have focused on the optimal design of the well locations in a pump and treat system.
The simulating-optimizing coupled method is one of the best methods for designing a groundwater pump and treat system. The simulation model primarily resolve the control equation of the groundwater flow and contaminant migration while optimization model is predominantly used for optimized the alternatives schemes [12-16]. The linear optimization method can solve plume-hydraulic control problem, but when the pollutant are set as the constraint conditions, a nonlinear optimization approach are needed [17-19]. The genetic algorithm (GA), which is a nonlinear mathematical optimization algorithm, is one of the most widely used methods. Huang and Mayer selected the well location as the discretization state variables and used the GA to optimize a groundwater remediation scheme in the pump and treat system [20]. Mahinthakumar and Sayeed solved the pollution source identification problem with a combined GA-Local Search method [21]. Gamze Gümüş-Demirci used the GA to analyze the effects of different crossover and mutation on the optimized result for a pump and treat system. They concluded that the efficiency of the GA depended on the code and cross plan when the decision variables were less [22].

Recently, optimization research on groundwater remediation has been conducted using the coupled simulation-optimization model. Jiabao Guan proved that a simulation-optimization model could effectively identify the position of nonlinear pollution sources and discharge history [23]. Thangjam Somchand Singh et al resolved the multi-objective optimization problem using a combined MODFLOW 2000-MT3DMS 5.0 and single-pass GA [24]. Sharief et al proved that the coupled Finite Element Method- Higher genetic algorithm (FEM-EGA) could efficiently repair a large aquifer by using a groundwater pump and treat system [25]. After research and comparison of various methods, we chose the Visual MODFLOW and MGO module to design an actual optimization project in an informal domestic waste landfill site.

2. Study area
The study area was located in the northeast suburb of a city in North China, and the sketch map was showed in figure 1. An informal landfill was located in the northwest part of the site which was used to dispose the household waste and garbage from livestock and poultry farming. The east of the site was sited a pig farm while both the west and the south side were cropland. The average temperature was 11.7℃. The annual precipitation was 575.5 mm with an unevenly distributed, and approximately 75% of the annual precipitation was mainly focused in the flood season. Atmospheric precipitation infiltration was the primary recharge sources in the study area while the groundwater runoff and regional groundwater exploitation were the main discharges. The evaporation capacity was slight and could be neglected due to the deep groundwater level.

![Figure 1. A sketch map of the study area.](image-url)
3. The construction of models

3.1. The construction of the hydrogeological concept model

Based on the drill data and water level data, the aquifer were primarily composed of fine sand with 6.97 meters deep averagely, and the water depth ranged from 20.00 meters to 21.20 meters. According to the monitoring data, water level remained primarily with 0.5 meter fluctuation. The aquifer was divided into a single homogeneous isotropic aquifer due to its smaller scale. Horizontal motion prioritized the groundwater flow, and vertical seepage could be neglected. Therefore, the groundwater flow could be treated as a two-dimensional unsteady flow and obeyed Darcy’s law. The boundary conditions were defined based on the contour of water table and the scope of the model domain after full consideration. The east and northwest borders were approximately perpendicular to the contour and there was no water exchange between boundaries. Therefore, the east and northwest boundary was defined as impervious theoretically. The northeast boundary was defined as constant flow boundary due to the fact that it was approximately parallel to the contour [26,27]. The definition of the boundary conditions were compatible with the real hydrogeological conditions, which ensured an accurate prediction in the subsequent simulation.

The hydrogeological parameters are the foundation of a groundwater numerical model. Traditional method to acquire the hydrogeological parameter consist of slug test and pump test [28]. We conducted slug test and pump test in the study area, and the result of the slug test indicated that the hydraulic conductivity of the site was 4.51 m/d, while the pump test showed the parameter was 4.37 m/d. The results were similar, and both were accordance with the empirical values for fine sand (1.5-5.0 m/d) [29]. Therefore, we could draw the conclusion that the two tests had a high accuracy. We chose the average value of 4.44 m/d as the initial value of the groundwater numerical model, and the final value could be determined by the result of model calibration. The influence radius of the pumping well was 12 meters based on the pumping test result, and the maximum pump rate was 67 m³/d calculated by Dupuit formula. The two parameters were determined from the result of pumping test and could characterize the hydrogeological characteristics of the study area.

3.2. The construction of the groundwater flow and solute transport model

The groundwater flow model was constructed based on the hydrogeological concept model. The model grid was divided into 50×60 cells and the cell size was 2 m×2 m. The site was considered with a homogeneous aquifer according to its hydrogeological characteristics. The initial value of the parameters was decided based on the formation lithology and the computation results of the pump and slug tests.

| Parameters               | Value | Parameters               | Value |
|--------------------------|-------|--------------------------|-------|
| Cell size /m             | 2     | Transversal dispersivity /m | 10    |
| Aquifer thickness /m     | 6.97  | Longitudinal dispersivity /m | 1     |
| Conductivity /m·d⁻¹      | 4.30  | Stress period /d         | 1     |
| Porosity                 | 0.2   | Time step /d             | 10    |
| Specific yield           | 0.18  | Retardation factor       | 1     |

By using the finite difference method, the initial simulation time was started on January 1, 2017, and ended on January 1, 2022. We set one month as a stress period, and the step size was ten in each stress period. The basic subroutine, calculate cell flow and recharge packages were required in groundwater flow model. The simulation results was verified by groundwater measured value in each month. The rapid convergence and stable preconditioned conjugate-gradient (PCG) solver were chosen in the groundwater flow model while the implicit GCG method in the solute transport model [30-32]. The concept model, the simulation scope, aquifer, source-sink term, and boundary conditions
of the solute model were treated as the same as groundwater flow model. The final model parameters after the calibration and adjustment were shown in Table 1.

High concentration of nitrate from household waste and garbage from livestock and poultry farming were the pollution sources. Nitrate was treated as a modeling factor with an infiltration concentration of 100 mg/L. Neglecting the influence of the temperature and water density change in the hydrodynamic and concentration fields, the simulation time was started on January 1, 2017. The nitrate pollution plume was simulated for five years based on natural groundwater flow, which was set as the initial plume for well layout optimization in pump and treat system. The initial plume was showed in Figure 2.

![Figure 2. The initial plume of the study area.](image)

3.3. Visual MODFLOW-MGO coupling model

3.3.1. The Optimization principle. The simulating-optimizing calculation were proceed by Visual MODFLOW-MGO coupling model. The groundwater flow were simulated by MODFLOW module while the solute transport were simulated by MT3DMS module. The pumping wells layout scheme were optimized by coupling the simulation results of groundwater flow and contaminants transport with MGO procedure.

The objective function of optimization computation in MGO procedure can be expressed as follows [33]:

$$J = \sum_{k=1}^{18} y_k Q_k \Delta t_k$$

Where, $J$ is the objective function in terms of the total amount of pumping water, m³; $Q_k$ is the pumping rate of the well $k$, m³/d; $y_k$ is a binary variable and equal to 1 if the well $k$ is active or 0 if the $k$ is inactive; $\Delta t_k$ is the pumping duration of well $k$, d.

GA was used to optimize the layout of the pump wells. The governance objective of the nitrates concentration was set as 20 mg/L on the baseline of human health. The value was suitable for drinking water meanwhile for industrial and agricultural water to achieve the groundwater quality standard III [34]. We assumed that the pollution source had been eliminated, thus the possibility of contamination...
infiltration to the target aquifer during the operation of the pump and treat system can be neglected. The constraint conditions consisted of the decision variables and state variables. The decision variables included the pumping rate and well location while the state variables consisted with the hydraulic head and concentration of each grid. The decision variables were defined as follows:

\[ 0 \leq Q_k \leq 67 \quad \text{and} \quad \sum_{i=1}^{n} y_i \leq n; \]

where \( Q_k \) was the pump rate of well \( k \); \( y_i \) was a binary variable equal to either 1 if parameter \( k \) was active (or 0 if parameter \( k \) was inactive); \( N \) was the total number of wells to be optimized. The state variable were defined as: \( C \leq C^* \), \( C^* \) is the target control concentration, which was set as 20 mg/L. The populations and the largest genetic iteration number of genetic algorithm were defined as 100. Meanwhile, the discretization interval number of pump rate of each well was defined as 32, and the crossover probability was 0.90 while the mutation probability was 0.05 to avoid the problem of convergence in genetic algorithm.

3.3.2. The overview of genetic algorithm principle. Genetic algorithm originated from computer simulation of biological systems and it was created by professor Holland and his students of University of Michigan. GA is fit to adaptive probability optimization of complex system and imitate the biological evolution of nature and genetic mechanism to achieve random global search and optimization. The individual undergoes generations of evolution, including choosing, crossing and variation operation, to achieve the constraint condition in counting process. GA is an efficient, parallel computing and global search stochastic algorithm and can automatically acquire and accumulate knowledge during search process to achieve optimal solution through control of the search adaptively. The calculation process of GA in MGO procedure was showed in figures 3 and 4.

4. Optimization calculation of the pumping scheme

4.1. The constant pumping rate scheme

Due to the long running period of the pump and treat system, the objective function was defined as minimum total pumping capacity. A series of candidate wells were set up as the initial conditions. The number of the initial candidate wells was 16, and these wells set up in the plume refer to relevant references. The candidate wells were shown in figure 5.

Combined with the actual hydrogeological and pollution conditions, the well numbers of 1, 2, and 3 were considered after the full economic analysis and applicable consideration. The well location, pumping rate and operation days were calculated using the GA in MGO procedure. The calculate results were shown in table 2.
Figure 4. The calculation process of GA in MGO procedure.

Figure 5. Candidate well locations.
Table 2. Calculate results at target governance time of 100 d.

| Number of pumping wells | Optimal well location | Single-well output /m³ | Optimal water output per day /m³ | Total output during the remediation time m³ |
|-------------------------|-----------------------|------------------------|----------------------------------|------------------------------------------|
| 1                       | PM6                   | 27.6                   | 27.6                             | 2,760                                     |
| 2                       | PM6, PM7              | 12.2, 12.2             | 24.4                             | 2,440                                     |
| 3                       | PM6, PM6, PM11        | 10.3, 10.3, 3.8        | 24.4                             | 2,440                                     |

As shown in table 2, the optimal water output per day with 2 or 3 wells scenario was less than 1 well scenario by approximately 11.6%. Therefore, multiple wells scenario may effectively reduce the total amount of the pumping water. A comparison of the 2 and 3 wells scenarios showed that the optimal water output per day was equivalent although the single well output was different. The scenario with 2 pumping wells was more reasonable than 3 wells in terms of the installation cost. Additionally, after optimizing the pumping wells, the result showed that the optimization scheme could save the installation cost of 14 wells compared with the initial condition.

Based on the well location of optimization scheme, it was concluded that the pumping well locations were not constrained by the well number and associated with the distribution of contaminate plume. The optimal scheme of pump wells were located near the central axis and in the middle and lower reaches of the plume. This kind of well layout scheme could effectively achieve the hydraulic control of the plume. The result showed that the optimum 2 wells were located about 5 meters far from the northern boundary of the study area as shown in figure 5.

![Figure 6. Optimal well location in 2 wells scenario.](image)

We also analyzed the optimal result of different target times in 2 wells scenario as shown in table 3. The initial target time was set as 100d, 75d and 50d. It was concluded from table 3 that reducing the target treatment time could increase the water output per day in the same remediation goal and well location. The total output during remediation time showed a high-low-high trend and the minimum water output was 1,980 m³ when the treatment management time was 75 days. It was reduced by 11.6% and 7.9% compared with the 100 days and 50 days of treatment time separately. Therefore, 75 days
was a reasonable treatment time in this site. We can concluded that PM6 and PM7 with the same pumping rate of 12.2 m$^3$/d and run for 75d were the optimal solution in constant pumping rate scheme.

**Table 3.** Optimal result of different target time in 2 wells scenario.

| Target time | Single-well output | Optimal water output per day m$^3$ | Total output during the remediation time m$^3$ |
|-------------|--------------------|-----------------------------------|---------------------------------------------|
|             | PM 6               | PM 7                             |                                             |
| 100 d       | 12.2               | 12.2                             | 22.4                                        | 2,240                                       |
| 75 d        | 13.2               | 13.2                             | 26.4                                        | 1,980                                       |
| 50 d        | 21.5               | 21.5                             | 43.0                                        | 2,150                                       |

The residual contaminant remains in the aquifer when the pumping well had run for 10 d, 25 d, 50 d, and 75 d were shown in figure 7. The residual quantity was 85%, 38% and 10% when the system had run for 10 d, 25 d and 50 d respectively with the constant pumping rate of 75 m$^3$/d. It was concluded that the pollutant concentration decreased quickly approximately before the system run for 25 days and we called it the first stage and after that the contaminant concentration decreased slowly due to the trailing effect. Therefore, setting up the two stages strategically can improve the pump and treat system efficiency, and meanwhile may reduce the groundwater contamination cost.

![Figure 7. Residual contaminant in different periods with a constant pumping rate.](image)

**4.2. The phased pumping rate scheme**

The phased pumping rate scheme was designed based on the optimal result of the constant scheme with the same well locations of PM6 and PM7. In the first stage, the pump rate of the two pumping wells increased by 50%, 100% and 200%, and the decision variable $t_1$ was determined from the model calculation. The decision variables $t_2$ and $Q_2$ were calculated on the basis of the first stage according to the GA.

The total output with different pumping rate with a treatment time of 75 days are showed in table 4. It can be inferred that the single well output increased by 50%, 100% and 200% compared with optimal result of constant scheme, the total outputs would reduce by approximately 15%, 9.8% and 0.1% respectively. The phased pumping method can effectively reduce the total output during the target management time.
Table 4. Comparison of the pump output with different pumping rate during the management time.

| Single-well output $Q_1$ (m³/d) | Single-well output $Q_2$ (m³/d) | The duration of the first stage $t_1$ (d) | The duration of the second stage $t_2$ (d) | Total output during the remediation time $Q$ (m³) |
|-------------------------------|-------------------------------|--------------------------------------|--------------------------------------|--------------------------------------|
| 19.8                          | 6.93                          | 25                                   | 50                                   | 1683                                 |
| 26.4                          | 8.3                           | 15                                   | 60                                   | 1785                                 |
| 59.4                          | 1.6                           | 9                                    | 66                                   | 1975                                 |

A comparison of the per well output and total output in the management time showed that simply increase the single well output in the first stage cannot effectively reduce the total output. It is necessary to perform a simulation when designing a phased pumping scheme. We can concluded that the pump schedule as $Q_1=19.8$ m³/d, $Q_2=6.93$ m³/d, $t_1=25$ d, $t_2=50$ d express the minimum total water output which was the optimal pumping scheme in phased pumping rate scheme. The total water output reduced 15% compared with the optimal pump scheme in constant pumping scheme.

The comparison of the residual contaminant of optimal pump scheme in the two pumping scheme were showed in figure 8. Due to the highly pumping rate in the first stage, the contaminate plume near the well was extracted quickly and indicated a large concentration gradient, which accelerated the pollution move to pump well. Therefore, the residual contaminant in phased pumping scheme was less compared with the constant pump rate scheme in the first stage. In the second stage, with a lower pumping rate of 6.93 m³/d due to the smearing effect can achieved the eliminate goal. Therefore, the phased pump rate scheme can effectively reduce the total output and improve the operation efficiency of the pump and treat system while bring considerable economic benefits.

![Figure 8. Residual contaminant of the constant pump rate scheme and phased pumping rate scheme.](image_url)

5. Conclusions
In this study, we used the Visual MODFLOW-MGO to optimize the pumping scheme in a heavily nitrate-polluted informal domestic waste landfill site in North China. The optimal scheme of pump wells were located near the central axis and in the middle and lower reaches of the plume which could effectively achieve the hydraulic control of the plume. The result can provide a good reference for pumping wells layout of contaminated site with similar hydrogeological condition.

After carefully calculate and compare the number of wells and the pumping capacity, we can concluded that PM6 and PM7 with the same pumping rate of 12.2 m³/d and run for 75d was the
optimal scheme in constant pumping rate scheme. Also, with the same well layout solution, the pump schedule as $Q_1=19.8 \text{ m}^3/\text{d}$, $Q_2=6.93 \text{ m}^3/\text{d}$, $t_1=25\text{d}$, $t_2=50\text{d}$ express the minimum total water output which was the optimal pumping scheme in phased pumping rate scheme. The total water output in phased pumping rate scheme reduced 15% compared with the optimal pump scheme in constant pumping scheme, which indicated that the phased pump rate scheme can effectively reduce the total output and improve the operation efficiency of the pump and treat system. However, in the condition of the aquifer was thin, the maximum pumping capacity of well was small or with limited sewage treatment capacity, the remediation time could be extend to achieve the remediation goals.

We divided the whole process of pumping into two stages in this study. However, in the actual remediation process, the changing condition of the pollutants in the groundwater are more complicated during the pumping process. Therefore, multi-stage simulation study are needed and the treatment time may be divided into several stages to simulate the remediation performance, which need a further research.

Acknowledgments

This research was financially supported by the National Key Research and Development program of China (2016YFE0102400).

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