Optimal design of cleanup schemes for groundwater polluted by multiple contaminants

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ABSTRACT

A formulation to design the optimal cleanup schemes for groundwater polluted by multiple contaminants of different characteristics is described. The objective function is a weighted sum of the volumes of the extracted and/or injected water. The groundwater quality constraints include, for each contaminant, the pointwise and the spatially averaged residual concentrations. Various solutions to a hypothetical problem involving two contaminants of different characteristics and remediation requirements are presented.

INTRODUCTION

Pump-and-treat is one of the major technologies employed for the remediation of contaminated groundwater aquifer systems. For cases when the remediation is targeted at a single contaminant, several formulations have been proposed to combine groundwater simulation models with optimization tools for the design of groundwater quality control schemes. Literature review can be found, for example, in the work by Culver and Shoemaker. In practice, the remediation requirements may not be limited to one single contaminant. When several contaminants are to be removed to restore the groundwater to specified quality levels, a desirable pumping scheme should be optimal for the simultaneous removal of all the targeted contaminants. Different contaminants may come from different sources and react with the porous media and each other in various ways. Such differences will influence the selection of optimal pumping schemes for cleanup.

This paper presents a formulation to determine the optimal pumping schemes for the removal of multiple contaminants. The solution to a hypothetical remediation problem involving two contaminants is presented and compared to cases in which only a single contaminant is targeted.
THE SIMULATION MODEL

Consider steady state groundwater flow and multiple contaminant transport in a vertically integrated confined aquifer system. The two-dimensional behavior are governed by the following equations

\[
\frac{\partial}{\partial x_i} \left( b K_{ij} \frac{\partial}{\partial x_j} h \right) = -\sum_{l} q_l \delta(x-x_l, y-y_l) - w(x_1, x_2) = (x, y) \in \Omega \tag{1}
\]

\[
v_i = -\frac{1}{\phi} K_{ij} \frac{\partial h}{\partial x_j} (x, y) \in \Omega \tag{2}
\]

\[
\left[ \frac{\partial}{\partial x_i} (\phi b D_{ij} \frac{\partial}{\partial x_j}) - \phi b v_i \frac{\partial}{\partial x_i} - b(\phi + \rho_b K_{\beta d}) \frac{\partial}{\partial t} - b \lambda_\beta (\phi + \rho_b K_{\beta d}) \right] c_\beta = -\sum_{l} q_l (c_{\beta i} - c_\beta) \delta(x-x_l, y-y_l) - w(c_{\beta i} - c_\beta) (x, y) \in \Omega, t \in [t_0, t_*] \tag{3}
\]

where, \( h[L] \) denotes the hydraulic head; \( c_\beta[ML^{-3}] \) concentration of the contaminant species \( \beta \); \( v_i[LT^{-1}] \) \( i \)th component of groundwater pore velocity; \( b[L] \) aquifer thickness; \( K_{ij}[LT^{-1}] \) tensor of hydraulic conductivities; \( D_{ij}[LT^{-2}] \) tensor of dispersion coefficients, function of \( v_i \) and the dispersivities \( \alpha_i \) and \( \alpha_t[L] \); \( \delta_{ij} \) Kronecker delta; \( \phi[L^3] \) porosity of the aquifer; \( \rho_b[ML^{-3}] \) soil bulk density; \( K_{\beta d}[L^3M^{-1}] \) partition coefficient for species \( \beta \); \( (x_l, y_l)[L] \) location of well \( l \); \( q_l[L^3T^{-1}] \) the injection(+) or extraction(-) rate of the well \( l \); \( c_{\beta i}[ML^{-3}] \) the concentration of species \( \beta \) in injected or extracted water by the well \( l \); \( \delta(x-x_l, y-y_l)[L^{-2}] \) Dirac delta function at \( (x_l, y_l) \); \( \lambda_\beta[T^{-1}] \) decay coefficient for species \( \beta \); \( w[LT^{-1}] \) the leakage flux into(+) or out of(-) the aquifer; \( c_{\beta i}[ML^{-3}] \) source distribution function for contaminant species \( \beta \); \( \Omega \) the aquifer domain; \( t_0 \) and \( t_* \) the starting and ending times of simulation.

The finite element versions of Equations (1) and (3) are

\[
A h = r \tag{4}
\]

\[
\left( H^\beta + G^\beta \frac{\partial}{\partial t} \right) c_\beta = s_\beta \tag{5}
\]

where, \( A, H^\beta \) and \( G^\beta \) are the coefficients matrices, \( r \) and \( s_\beta \) the vectors of driving forces for flow and transport, and \( h \) and \( c_\beta \) the vectors of hydraulic heads and contaminant concentrations.

THE OPTIMIZATION FORMULATION

Define a decision vector of pumping rates as \( d = [q_1^+ q_1^- \cdots q_n^+ q_n^-]^T \), with \( n \) being the total number of potential remediation wells, and \( q_i^+ \) and \( q_i^- \) the injection and extraction rates at the potential well node \( i \). Note that the actual pumping rate at node \( i \) can be expressed as \( q_i = q_i^+ - q_i^- \) on
the condition that the physical constraint keeps at least one of the two components of $q_i$ as zero. The following optimization formulation is utilized to determine the optimal pumping scheme for the simultaneous removal of the various targeted contaminants,

$$\min (t_s - t_0) \sum_{i=1}^{n} (\alpha^+ q_i^+ + \alpha^- q_i^-)$$

(6)

$$0. \leq q_i^+ \leq \bar{q}_i^+ , \quad 0. \leq q_i^- \leq \bar{q}_i^- \quad i = 1 \sim n$$

(7)

$$0. \leq \sum_{i=1}^{n} q_i^+ \leq q_{max}^+ , \quad 0. \leq \sum_{i=1}^{n} q_i^- \leq q_{max}^-$$

(8)

$$\sum_{i=1}^{n} q_i^+ q_i^- = 0. \quad (9)$$

$$\dot{c}_{\beta \xi}(q^+, q^- ; t_s) \leq c_{\beta \xi}^* \quad \forall \beta \quad \forall \xi \quad (10)$$

$$c_{\beta j}(q^+, q^- ; t_s) \leq c_{\beta j}^* \quad \forall \beta \quad \forall j \quad (11)$$

where, $\alpha^+$ and $\alpha^-$ are the weighting factors with respect to the volume of injected water and the volume of extracted water respectively; $q^+$ and $q^-$ are n-vectors with $q_i^+$ and $q_i^-$ as the typical elements; $\bar{q}_i^+$ and $\bar{q}_i^-$ are the upper bounds on the injection and extraction rates for the potential well $i$, and $q_{max}^+$ and $q_{max}^-$ the allowable total injection and extraction rates respectively. $\xi$ stands for the aquifer zone in which the average residual contaminant concentration $\dot{c}_{\beta \xi}$ needs to be reduced to the specified level $c_{\beta \xi}^*$. $c_{\beta j}^*$ represents the allowable contaminant concentration for node $j$ at $t_s$. The type of constraint described by Equation (10) is specifically devised to design cleanup schemes, while the constraint type described by Equation (11) is most suitable for pointwise groundwater quality control.

The optimization package NPSOL developed by Gill et al. is employed to solve the above optimization problem. A state sensitivity method is used to compute the gradients. Equations (4) and (5) can be partitioned by considering Dirichlet and non-Dirichlet sets of nodes denoted by the subscripts ’c’ and ’u’ respectively. Taking the derivative of the non-Dirichlet portions of the equations with respect to the $k$th element of the decision vector $d$, we have

$$A_{uu} \frac{\partial h_u}{\partial d(k)} = \frac{\partial r_u}{\partial d(k)} - \frac{\partial A_{uc}}{\partial d(k)} h_u - \frac{\partial A_{uu}}{\partial d(k)} h_u$$

(12)

$$(\omega \Delta t_i H_{uu}^\beta + G_{uu}^\beta) \frac{\partial c_{\beta u}^{l+1}}{\partial d(k)} = - (\omega \Delta t_i \frac{\partial H_{uu}^\beta}{\partial d(k)} + \frac{\partial G_{uu}^\beta}{\partial d(k)}) c_{\beta u}^{l+1}$$

$$\quad + [-(1 - \omega) \Delta t_i H_{uu}^\beta + G_{uu}^\beta] \frac{\partial c_{\beta u}^l}{\partial d(k)} + [-(1 - \omega) \Delta t_i \frac{\partial H_{uu}^\beta}{\partial d(k)} + \frac{\partial G_{uu}^\beta}{\partial d(k)}] c_{\beta u}^l$$
where finite differencing has been used for temporal variations; and \( l, \Delta t \) and \( \omega \) denote the time step, step length and the weighting factor respectively.

**AN EXAMPLE**

Various solutions to a hypothetical problem involving two contaminant species are presented. Figure 1 shows the physical domain and the flow boundary conditions. For contaminant transport, zero-concentration is assumed for the \( h = 104m \) part of the boundary, and zero-concentration-gradients are assumed for other boundary parts. Assume that the aquifer is confined above by a leaky aquitard and below by an impermeable layer. Both the aquifer and the aquitard have uniform thicknesses, and are isotropic and homogeneous. The aquifer properties are given in Table 1. The relevant aquitard properties are: hydraulic conductivity 0.0005m/day, thickness 2.0m, and the hydraulic head above the aquitard 108m. The two contaminant species, with source concentrations \( c_1^0 = 500 \) and \( c_2^0 = 1000 \) (in mass unit/m\(^3\)) respectively, migrated in the natural hydraulic field for 700days at which time the sources were cutoff. The resulting concentrations shown in Figures 2 and 3, with average concentrations of 0.426 and 0.283 mass units/m\(^2\) respectively, are taken as the initial contaminant plumes for the remediation. The properties of the contaminants are presented in Table 2. Also shown in Figure 3 are the locations of the assumed potential remediation wells. Listed in Table 3 are the parameters for the optimization formulation. Assume \( \alpha^\pm = 1.0 \) and \( t_\text{s} = 400\text{days} \). The cleanup requirements are to reduce the contaminant concentrations averaged over the entire domain to the specified values of \( c_1^* \) and \( c_2^* \).

As an illustration, the marginal sensitivities of \( \hat{c}_{\beta_\ell} \) with respect to \( q_{i_\ell}^+ \) at \( t = 400\text{days} \) is plotted in Figure 4. Note that the lines connecting the data points are plotted merely for reading convenience. Figure 5 presents the optimal pumping schemes when different species are targeted by the optimization. The corresponding remediation effects are given in Figure 6. Despite the fact that the optimization formulation allows injection wells, the optimal solutions are found to be purely extraction pumping. In case (b), both contaminant species are explicitly targeted, with 10 wells being selected to meet the cleanup requirements. Case (a) gives the solution when only the species \#1 is targeted; 11 wells are selected with the total pumping rate being smaller than that in case (b). Case (c) is the solution when only the species \#2 is targeted; only 6 wells are found to be active and the total pumping is the smallest of all the cases considered. Although the optimal solution is primarily influenced by the \#1 contaminant plume, the requirement for species \#2 cannot be satisfied by targeting only at species
With respect to the optimization, the differences between the two contaminants are the initial plumes, partition properties and the quality requirements. Generally, the optimal pumping scheme for the simultaneous remediation of both contaminants can only be determined by explicitly specifying the quality requirements for both contaminants.

<table>
<thead>
<tr>
<th>Table 1: Properties of Aquifer</th>
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<tr>
<td>$K (m/day)$</td>
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<td>120</td>
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<table>
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<th>Table 2: Properties of Contaminants</th>
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<tr>
<td>species #1</td>
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<tr>
<td>$\lambda_1 (1/day)$</td>
</tr>
<tr>
<td>$K_{1d} (m^3/mass \ unit)$</td>
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<th>Table 3: Parameters for Optimization</th>
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<tr>
<td>$\bar{q}_i^+ (m^3/day)$</td>
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<tr>
<td>7000</td>
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**SUMMARY**

This paper described an optimization formulation which is suitable to determine the optimal pumping schemes for the simultaneous removal of multiple contaminants in a contaminated groundwater aquifer system. To demonstrate the formulation, various solutions to a hypothetical problem involving two contaminants of different characteristics and remediation requirements were presented.

**REFERENCES**


Figure 3: The initial concentrations of species #2

Figure 4: $z = \partial c_\beta / \partial q_i^+ \text{ at } q_i^+ = 0 \text{ and } t = 400\text{days}$
Figure 5: Optimal pumping schemes when (a) species #1 is targeted, (b) both species #1 and #2 are targeted, and (c) species #2 is targeted.

Figure 6: Remediation effects when (a) species #1 is targeted, (b) both species #1 and #2 are targeted, and (c) species #2 is targeted.