Supplemental Information to Accompany "Optimal Design for Problems Involving Flow and Transport Phenomena in Saturated Subsurface Systems"

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Abstract

Following is supplemental information to accompany "Optimal Design for Problems Involving Flow and Transport Phenomena in Saturated Subsurface Systems." This material consists of details necessary to execute the Community Problems discussed in the subject article.

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Notation

Roman Letters

b_j	exponential coefficients in cost objective functions
c_j	coefficients in cost objective functions
C_0^ι	initial contaminant distribution for species ι
C_s^ι	source or steady state concentration for species ι
C^{sw}	concentration of solute in seawater
C_b^ι	background concentration of solute in freshwater
C_i^ι	concentration in extraction well i for species ι
C_E^ι	target effluent concentration from treatment process for species ι
$\overline{C}^\iota$	design influent concentration for treatment process for species ι
$\mathbf{D}$	hydrodynamic dispersion tensor
$D^{\iota*}$	free liquid diffusivity of species ι
d_i	depth of well below the ground surface
f	objective function
f^c	capital costs
f^o	operational costs
F_{sw}	allowable solute concentration normalized by seawater concentration
g	magnitude of gravitational acceleration, oriented in the $-\mathbf{k}$ direction
h	hydraulic head
h^{max}	maximum allowable head
h^{min}	minimum allowable head
h_i	head in well i
h_s	steady-state solution to the unperturbed flow problem
H^ι	Henry's law coefficient for species ι
$\mathcal{I}$	interphase mass exchange
$\mathcal{I}^\iota$	interphase mass transfer relations
k	scalar intrinsic permeability
$\mathbf{k}$	effective permeability tensor
$\mathbf{K}$	hydraulic conductivity tensor
K	hydraulic conductivity scalar
k_f	first-order mass transfer rate coefficient
K_f	Freundlich capacity coefficient
M	maximum fractional mass remaining after remediation
n	number of wells
n^e	number of extraction wells
n_f	exponent related to the sorption energy
n^i	number of injection wells
$\mathbf{q}$	Darcy velocity, or volumetric flux
p	fluid pressure
q_y, q_z	Darcy flux out of the domain
Q_i^m	design extraction rate at well i

Q^{emax}	maximum extraction rate
Q^{imax}	maximum injection rate
Q_T	total net pumping rate rate
Q_T^e	total extraction rate
Q_T^{max}	maximum total extraction rate
Q_T^{min}	minimum total extraction rate
Q_i	extraction or injection rate for well i
	$Q_i < 0$ indicates extraction and $Q_i > 0$ indicates injection
r	species qualifier for the sorbing species
R	treatment process removal efficiency
$\mathcal{R}^\iota$	biogeochemical reactions
S_s	specific storage coefficient
$\mathcal{S}$	solute source term
$\overline{\mathcal{S}}$	fluid source term
t	time
t_f	operation or remediation time
t_s	plume development time
$\mathbf{v}$	mean pore fluid flow velocity vector
$\mathbf{x}$	position vector
$\mathbf{x_s}$	location of contaminant source
$\mathbf{x_i}$	well locations
z	spatial coordinate oriented aligned with $\mathbf{k}$
z_{gs}	elevation of ground surface
Z	height of air stripping tower

Greek Letters

α_l	longitudinal dispersivity
α_t	transverse dispersivity
η_x, η_y, η_z	spatial correlation scales
μ	dynamic viscosity of the aqueous phase
$\mu_{\log K}$	mean K in $\log_{10}$ space
ν, ν_x, ν_y, ν_z	spatial coordinates in covariance model
ω	mass fraction
Ω	model domain
ρ	density of the aqueous phase
ρ_0	freshwater density
ρ_{sw}	seawater density
$\sigma_{\log K}^2$	variance of K in $\log_{10}$ space
τ	tortuosity of the porous medium
θ	volume fraction

Subscripts

i	well index
s	qualifier denoting source or steady state

Superscripts

a	qualifier denoting aqueous phase
e	qualifier denoting extraction
i	qualifier denoting injection
s	qualifier denoting solid phase
ι	species index

1 Applications

A set of four applications (I–IV) is listed in Table 1 along with corresponding entries for possible choices of domains, model formulations, objective functions, and constraints, the details of which are included in the sections that follow. The applications considered are: a well-field design, well-field design with seawater intrusion, the capture of a contaminant plume, and PAT remediation of a contaminant plume(s). The domains include a range of homogeneous and heterogeneous systems. The models include mathematical representations of fluid flow and contaminant transport in confined and unconfined aquifers. The objective of all problems is to minimize the cost of the installation and operation of a set of wells. In addition, the PAT application includes a treatment cost component. Decision variables include the number (n), location $(\mathbf{x}_i; i = 1, \ldots, n)$, and pumping rates (Q_i) for all wells. Constraints include bounds on individual and total pumping rates and heads.

The problem specifications are outlined to allow latitude in approaching the design problem. For example, well locations and numbers can be arbitrary or selected from a specified candidate set. Further, pumping rates can be taken as constant, constant over intervals, or follow some user-specified function.

2 Domains

Five domains are summarized in Table 2 according to a general description and properties of a scalar K, which distinguishes these domains. The spatial domain for all cases is $\Omega \in [0, 1000] \times [0, 1000] \times [0, 30]$ m.

Table 1
Community Application Designs

Application	Description	Domains	Models	Objectives	Constraint Equations
I	well-field	A–E	1 & 2	a	(39)–(41)
II	well-field/ sea-water intrusion	A–E	3	a	(39)–(42)
III	capture zone	A–E	2	a	(39)–(41), (43), (*)
IV	pump-and-treat	A–E	4 & 5	b	(39)–(41), (43), (44)

* capture constraint is specified by initial plume configuration

Table 2
Problem Domains

Domain	Description	$\mu_{\log K}$	$\sigma^2_{\log K}$	η_x, η_y, η_z
A	homogeneous	-4.3	NA	NA
B	layered	-4.3	1	NA
C	random field I	-4.3	1	5, 5, 0.75
D	random field II	-4.3	2	5, 5, 0.75
E	random field III	-4.3	1	50, 50, 7.5

Note: log refers to $\log_{10}$

The medium properties are homogeneous for Domain A, with $K = 5.01 \times 10^{-5}$ m/s. For Domain B, the domain consists of 10 layers of equal thickness with K described as uniform in each layer, log-normally distributed, and uncorrelated in space. The K distribution for Domain B can be downloaded by following the instructions given at the end of the web page. For Domains C–E, K is a correlated random field following a normal distribution in log-transformed space where $\mu_{\log K}$ and $\sigma^2_{\log K}$ are the mean and variance of K in $\log_{10}$ space. K is spatially correlated according to the exponential covariance model

$$\mathrm{cov}(\nu) = \sigma^2_{\log K} \exp\left(-\sqrt{\frac{\nu_x^2}{\eta_x^2} + \frac{\nu_y^2}{\eta_y^2} + \frac{\nu_z^2}{\eta_z^2}}\right) \tag{1}$$

where ν, ν_x, ν_y, and ν_z are spatial coordinates and η_x, η_y, and η_z are spatial correlation scales in the x, y, and z directions. Domains C and D differ from each other in the value of log K variance, $\sigma^2_{\log K}$. Domains C and E differ from each other in the value of the correlation scales η_x, η_y, and η_z. The K distribution for Domains C–E can be downloaded by following the instructions

given at the end of the web page.

3 Mathematical Models

A variety of mathematical models are summarized in Table 3, which may be applied to approximate the applications outlined in Table 1. We specify the models in mathematical form only, so as not to preclude a given simulator. The models are based on saturated flow and/or transport models, which can be formulated for fluid flow by

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (K \nabla h) + \overline{\mathcal{S}} \tag{2}$$

and for species transport by

$$\frac{\partial(\theta^a C^\iota)}{\partial t} = \nabla \cdot (\theta^a \mathbf{D}^\iota \cdot \nabla C^\iota) - \nabla \cdot (\mathbf{q} C^\iota) + \mathcal{I}^\iota + \mathcal{R}^\iota + \mathcal{S}^\iota \tag{3}$$

where S_s is a specific storage coefficient, h is hydraulic head, t is time, $\overline{\mathcal{S}}$ is a fluid source term, θ^a is the aqueous phase volumetric fraction (= porosity), C^ι is the aqueous phase concentration of species ι, $\mathbf{D}$ is a hydrodynamic dispersion tensor, $\mathbf{q}$ is the Darcy velocity (specific discharge) vector, $\mathcal{I}^\iota$ represents inter-phase mass transfer relations, $\mathcal{R}^\iota$ represents biogeochemical reactions, and $\mathcal{S}^\iota$ represents a source of mass.

Darcy's law is used to approximate momentum conservation:

$$\mathbf{q} = \theta^a \mathbf{v} = -\frac{k}{\mu} (\nabla p + \rho g \nabla z) \tag{4}$$

where $\mathbf{v}$ is the mean pore velocity; k is the intrinsic permeability of the porous medium ; μ is the dynamic viscosity of the aqueous phase; p is the fluid pressure of the aqueous phase; ρ is density of the aqueous phase; g is the magnitude of gravitational acceleration, which is assumed to be oriented in the -$\mathbf{k}$ direction, and z is a spatial coordinate oriented aligned with $\mathbf{k}$.

The dispersion tensor is written as

$$\mathbf{D}^\iota = D_{ij}^\iota = \delta_{ij} \alpha_t |\mathbf{v}| + (\alpha_l - \alpha_t) \frac{v_i v_j}{|\mathbf{v}|} + \delta_{ij} \tau D^{\iota*} \tag{5}$$

where α_l and α_t are the longitudinal and transverse dispersivities, respectively, τ is the tortuosity of the porous medium, and $D^{\iota*}$ is the free liquid diffusivity

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of species ι.

The set of decision variables, n, Q_i, and $\mathbf{x}_i$, enter through specification of $\overline{\mathcal{S}}$ and $\mathcal{S}^\iota$, which provide a mechanistic link to the state variables such that

$$\int_\Omega \overline{\mathcal{S}}(t)\,\mathrm{d}\Omega = \sum_{i=1}^n Q_i(\mathbf{x}_i, t) \tag{6}$$

$$\int_\Omega \mathcal{S}^\iota(t)\,\mathrm{d}\Omega = \sum_{i=1}^n Q_i(\mathbf{x}_i, t) C_i^\iota(\mathbf{x}_i, t) \tag{7}$$

where Ω is the domain of the system; Q_i is a volumetric rate of extraction or injection; and C_i^ι is a concentration of the fluid added to or removed from the system. Note that $Q_i < 0$ indicates extraction and $Q_i > 0$ indicates injection.

Model 1 follows eqn (2), as applied to confined single-phase flow. The auxiliary conditions for Model 1 are

$$\left.\frac{\partial h}{\partial x}\right|_{x=0} = \left.\frac{\partial h}{\partial y}\right|_{y=0} = \left.\frac{\partial h}{\partial z}\right|_{z=0} = 0 \; , \; t > 0 \tag{8}$$

$$q_z(x, y, z = 30, t > 0) = -1.903 \times 10^{-8} \; (\mathrm{m/s}) \tag{9}$$
$$h(x = 1000, y, z, t > 0) = 50 - 0.001y \; (\mathrm{m}) \tag{10}$$
$$h(x, y = 1000, z, t > 0) = 50 - 0.001x \; (\mathrm{m}) \tag{11}$$
$$\overline{\mathcal{S}}(x, y, z, t > 0) = 0.0 \tag{12}$$
$$h(x, y, z, t = 0) = h_s \tag{13}$$

where q_z is the Darcy flux out of the domain, h_s represents the steady-state solution to the flow problem in the absence of additional sources and sinks provided by a specified design, and $S_s = 10^{-6} \; (1/\mathrm{m})$.

Model 2 is similar to Model 1 but applies eqn (2) to an unconfined flow system with the auxiliary conditions given as

$$\left.\frac{\partial h}{\partial x}\right|_{x=0} = \left.\frac{\partial h}{\partial y}\right|_{y=0} = \left.\frac{\partial h}{\partial z}\right|_{z=0} = 0 \; , \; t > 0 \tag{14}$$

$$q_z(x, y, z = h, t > 0) = -1.903 \times 10^{-8} \; (\mathrm{m/s}) \tag{15}$$
$$h(x = 1000, y, z, t > 0) = 20 - 0.001y \; (\mathrm{m}) \tag{16}$$
$$h(x, y = 1000, z, t > 0) = 20 - 0.001x \; (\mathrm{m}) \tag{17}$$
$$\overline{\mathcal{S}}(x, y, z, t > 0) = 0.0 \tag{18}$$
$$h(x, y, z, t = 0) = h_s \tag{19}$$

where $S_s = 2 \times 10^{-1} \; (1/\mathrm{m})$, representing the specific yield of the unconfined aquifer. In Models 1 and 2, it is assumed that water is released from storage

instantly with a change in head.

Model 3 is appropriate for simulating seawater intrusion, and involves unconfined flow, eqn (2), and conservative species transport, eqn (3). Density dependence is considered via a concentration-dependent expression

$$\rho = \rho_0 + \frac{\partial \rho}{\partial C^\iota}(C^\iota - C_b^\iota) \tag{20}$$

where ρ_0 is the density of freshwater at the reference temperature, which is assumed to be time and space invariant, $\partial \rho / \partial C^\iota$ is the change in density with respect to solute concentration, and C_b^ι is the background concentration of solute in the freshwater, taken as $C_b^\iota \approx 0$. The specific storage in eqn (2) is adjusted for changes in density by a linear approximation: $S_s = [2 \times 10^{-1}(\rho/\rho_0)]$ (1/m).

The auxiliary conditions for Model 3 are

$$\left.\frac{\partial h}{\partial x}\right|_{x=0} = \left.\frac{\partial h}{\partial x}\right|_{x=1000} = \left.\frac{\partial h}{\partial z}\right|_{z=0} = 0 , \ t > 0 \tag{21}$$

$$p(x, y = 0, z, t > 0) = \rho_{sw} g z \tag{22}$$

$$q_y(x, y = 1000, z, t > 0) = -1.282 \times 10^{-5} \ (\text{m/s}) \tag{23}$$

$$h(x, y, z, t = 0) = h_s \tag{24}$$

$$\left.\frac{\partial C^\iota}{\partial x}\right|_{x=0} = \left.\frac{\partial C^\iota}{\partial x}\right|_{x=1000} = \left.\frac{\partial C^\iota}{\partial z}\right|_{z=0} = \left.\frac{\partial C^\iota}{\partial z}\right|_{z=h} = 0 , \ t > 0 \tag{25}$$

$$C^\iota(x, y = 0, z, t > 0) = C^{sw} , \ t > 0 \tag{26}$$

$$C^\iota(x, y = 1000, z, t > 0) = 0 , \ t > 0 \tag{27}$$

$$C^\iota(x, y, z, t = 0) = C_0^\iota(x, y, z) \tag{28}$$

where ρ_{sw} is the density of seawater, C_{sw}^ι is the concentration of solute in seawater ($C_{sw}^\iota = 35$ kg/m^3), and C_0^ι represents the steady-state solution to the solute transport problem in the absence of additional sources and sinks provided by a specified design. Table 4 lists the parameter values for Model 3.

Models 4 and 5 are appropriate for species transport as described by eqn (3) and the auxiliary conditions given as

$$\left.\frac{\partial C^\iota}{\partial x}\right|_{x=0} = \left.\frac{\partial C^\iota}{\partial y}\right|_{y=0} = \left.\frac{\partial C^\iota}{\partial z}\right|_{z=0} = \left.\frac{\partial C^\iota}{\partial z}\right|_{z=h} = 0 , \ t > 0 \tag{29}$$

$$C^\iota(x = 1000, y, z, t > 0) = C^\iota(x, y = 1000, z, t > 0) = 0 \tag{30}$$

$$C^\iota(x, y, z, t = 0) = C_0^\iota(x, y, z) \tag{31}$$

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where $C_0^\iota(x, y, z)$ is the initial contaminant distribution. The unperturbed (no pumping) flow fields for Models 4 and 5 are provided by the unconfined flow Model 2 applied to a choice from the set of possible Domains A–E. Applications III and IV require initial contaminant plumes that are expected to be captured or remediated. The initial concentration field, C_0^ι, may be generated by simulating plume development from a finite source for $t \in [-t_s, 0]$; for details see Table 5.

In Model 4, a single, conservative species ($\iota = c$) is considered, such that $\mathcal{I}^c = 0$ and $\mathcal{R}^c = 0$. This model is used to generate the plume to be captured in Application III and remediated in Application IV. Table 5 lists the parameter values for Model 4.

In Model 5, a conservative ($\iota = c$) and a sorbing ($\iota = r$) species are considered, C^c and C^r, respectively. Model 5 is to be used with Application IV. For the sorbing species, aqueous-solid phase mass exchange is described by a first-order rate model

$$\mathcal{I}^r = \theta^s \rho^s k_f \left(\omega^{rse} - \omega^{rs} \right) \tag{32}$$

where the Freundlich equilibrium model describes the relationship between the solid phase mass fraction and the fluid phase concentration at equilibrium

$$\omega^{rse} = K_f \left(C^r \right)^{n_f} \tag{33}$$

where r is a species qualifier for the sorbing species, k_f is a first-order mass transfer rate coefficient, ω^{rse} is the solid-phase mass fraction in equilibrium with the fluid-phase concentration, ω^{rs} is the solid-phase mass fraction, K_f is a Freundlich capacity coefficient, and n_f is an exponent related to the sorption energy. A separate mass balance equation for the mass fraction of the species sorbed to the solid phase must be solved,

$$\frac{\partial \omega^{rs}}{\partial t} = k_f \left(\omega^{rse} - \omega^{rs} \right) \tag{34}$$

in addition to solving the solute species mass balances. Table 5 lists the parameter values for Model 5.

4 Objective Functions

The objective function for each application is indicated in Table 1 and includes a capital cost f^c and an operational cost f^o, which depends upon

Table 3
Model Formulations

Model	Description	Model Equations
1	confined flow	(2), (8)–(13)
2	unconfined flow	(2), (14)–(19)
3	unconfined, density-dependent flow/conservative species transport	(2)–(5), (14)–(28)
4	unconfined flow/conservative species transport	(2)–(5), (14)–(19), (29)–(31)
5	unconfined flow/conservative and retarded species transport	(2)–(5), (14)–(19), (29)–(34)

Table 4
Parameters for Model 3

Parameter [Reference]	Value	Units
freshwater density, ρ_0 [4]	9.98×10^2	kg/m^3
seawater density, ρ_{sw} [4]	1.025×10^3	kg/m^3
seawater concentration, C^ι_{sw} [4]	3.5×10^1	kg/m^3
density dependence factor, $\partial\rho/\partial C^\iota$ [4]	7.7×10^{-1}	(kg/m^3)/(kg/m^3)
longitudinal dispersivity, α_l	1	m
transverse dispersivity, α_t	0.1	m
molecular diffusion, $D^{\iota*}$ [4]	6.6×10^{-6}	m^2/s
tortuosity, τ	0.4	-

time. The generic objective is to minimize the sum of $f^c + f^o$. The objective function for all applications and models depends upon the number, location, and extraction/injection rate of all wells. This amounts to specification of $Q_i(\mathbf{x}_i, t)$, $i = 1, \ldots, n$. The set of $\{\mathbf{Q}\}$ are ordered such that the extraction rates are $Q_i < 0$, $i = 1, \ldots, n^e$ and the injection rates are $Q_i > 0$, $i = n^e + 1, \ldots, n$, where n^e is the number of extraction wells, and the number of injection wells is $n^i = n - n^e$.

The capital cost for a well includes the well construction and, for the case of an extraction well, the cost of a pump. Injection wells are assumed to discharge

Table 5
Parameters for Models 4 and 5

Parameter [Reference]	Value	Units
source concentration*, $C_s^\iota(\mathbf{x}_s)$ $\iota = c, r$	1, $-t_s \le t \le 0$ 0, $t > 0$	kg/m^3 kg/m^3
plume development time, t_s	1.58×10^8	s
source location, $\mathbf{x}_s =$ $[(x_{s1}, x_{s2}); (y_{s1}, y_{s2}); (z_{s1}, z_{s2})]$	[(200,225);(475,525); (h-2,h)]	m
longitudinal dispersivity , α_l	1	m
transverse dispersivity, α_t	0.1	m
molecular diffusion, $D^{\iota *}$	10^{-9}	m^2/s
tortuosity, τ	0.4	-
Freundlich capacity coefficient, K_f [5]	3.34×10^{-5}	(kg/kg)/(kg/m^3)^{n_f}
Freundlich exponent, n_f [5]	0.70	-
mass transfer rate coefficient, k_f [3]	3.06×10^{-7}	1/s
aqueous volumetric fraction, θ^a	0.32	-
solid phase (particle) density, ρ^s	2.6×10^3	kg/m^3

*Note: it is assumed that the initial solid phase mass fraction is in equilibrium with the aqueous phase in the vicinity of the source.

under gravity feed conditions. The functional form for the capital cost is

$$f_a^c = \sum_{i=1}^{n} c_0 d_i^{b_0} + \sum_{i=1}^{n^e} c_1 |Q_i^m|^{b_1} (z_{gs} - h^{min})^{b_2} \tag{35}$$

and the operational cost is

$$f_a^o = \int_0^{t_f} \left(\sum_{i=1}^{n^e} c_2 Q_i (h_i - z_{gs}) + \sum_{i=n^e+1}^{n} c_3 Q_i \right) \mathrm{d}t \tag{36}$$

where b_j and c_j are coefficients and exponents of the cost model, respectively; d_i is the depth of the well below ground surface, Q_i^m is the design pumping rate, z_{gs} is the ground surface elevation, h^{min} is the minimum allowable head,

Table 6
Objective Functions

f forms	Description	Equations
a	installation + extraction + injection	$f_a = f_a^c + f_a^o$ (35), (36)
b	installation + extraction + injection + treatment	$f_b = f_b^c + f_b^o$ (37), (38)

t_f is the total time of operation, h_i is the hydraulic head in each well.

For the PAT application, the objective function includes not only the well construction and operation costs but also capital and operational costs related to treatment. We base our treatment cost functions on a cost model for air stripping resulting in the capital cost function

$$f_b^c = f_a^c + c_4 Z \tag{37}$$

and the operational cost function

$$f_b^o = f_a^o + \int_0^{t_f} Z \left(c_5 - c_6 Q_T^e \right) \, \mathrm{d}t \tag{38}$$

where Z is the total height of the stripping tower required, and $Q_T^e = \sum_{i=1}^{n^e} Q_i$ is the total extraction rate. The coefficients and accompanying equations associated with the objective functions are found in Table 7.

5   Constraints

The objective functions listed in Table 6 are constrained by hydraulic and solute mass constraints. For Applications I and II there are constraints on the total extraction rate due to the well-field demand, the extraction and injection rate at each well, and the aquifer drawdown

$$Q_T \leq Q_T^{min} \tag{39}$$

$$Q^{emax} \leq Q_i \leq Q^{imax}, \ i = 1, \ldots, n \tag{40}$$

$$h^{max} \geq h_i \geq h^{min} \ i = 1, \ldots, n \tag{41}$$

where $Q_T = \sum_{i=1}^{n} Q_i$ is the net pumping rate, Q_T^{min} is the minimum total extraction rate, Q^{emax} is the maximum extraction rate at any well, Q^{imax} is

the maximum injection rate at any well, h^{max} is the maximum allowable head, and h^{min} is the minimum allowable head.

For Application II an additional constraint is specified for the maximum solute concentration in the extraction wells

$$\frac{C_i^\iota}{C_{sw}^\iota} \leq F_{sw} \quad i = 1, \ldots, n^e \tag{42}$$

where C_i^ι is the solute concentration at extraction well i, and F_{sw} is the maximum allowable normalized solute concentration.

For Application III, we also constrain the total net extraction rate

$$\sum_{i=1}^{n} Q_i \geq Q_T^{max} \tag{43}$$

where Q_T^{max} is the maximum total extraction rate. The plume capture constraint is specified by the boundary of the initial contaminant distribution for each model domain. We leave it to the modeler to choose the physical and mathematical representation of the constraint (e.g. advective control vs. gradient control).

Application IV requires a constraint specifying the aquifer cleanup performance. To provide a common metric, we constrain the maximum global fraction of mass that may remain in the system at a time t_f, which is possible to do for the numerical studies of interest here but difficult to measure in practice. The fractional mass remaining constraint is

$$\frac{\int_\Omega \left(\theta^a C^\iota + \theta^s \rho^s \omega^{\iota s}\right)_{t=t_f} \mathrm{d}\Omega}{\int_\Omega \left(\theta^a C^\iota + \theta^s \rho^s \omega^{\iota s}\right)_{t=0} \mathrm{d}\Omega} \leq M \tag{44}$$

where M is the maximum fractional mass remaining at time t_f. When $\iota = c$ the solute mass on the solid-phase contribution is identically zero. However, when $\iota = r$ sorption to the solid phase must be accounted for when computing the fractional mass remaining in the system. The parameter values and associated with the constraints are found in Table 8.

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Table 7
Objective Function Coefficients and Equations

Coefficient/Equation [Reference]	Value/Function	Units
installation cost [2]*	$c_0 = 5.5 \times 10^3$	$/m^{b_0}$
	$c_1 = 5.75 \times 10^3$	$/[(m^3/s)^{b_1} \cdot m^{b_2}]$
	$b_0 = 0.3$	-
	$b_1 = 0.45$	-
	$b_2 = 0.64$	-
ground surface	$z_{gs} = 60$ Model 1	m
elevation	$z_{gs} = 30$ Model 2	m
extraction & injection well depth	$d_i = z_{gs}$	m
extraction cost [2]*	$c_2 = 1.05$	$/[(m^3/s) \cdot m \cdot s]$
injection cost [2]*	$c_3 = 0.56$	$/[(m^3/s) \cdot s]$
treatment capital cost [1]*	$c_4 = 2.5 \times 10^4$	$/m
treatment operating	$c_5 = 4.2 \times 10^{-5}$	$/(s \cdot m)$
cost [1]*	$c_6 = 9.0 \times 10^{-4}$	$/[s \cdot (m^3/s) \cdot m]$
air stripping tower height [1]	$Z = b_3 (H^\iota)^{b_4} |Q_T^e|^{b_5} R^{b_6} (\overline{C}^\iota)^{b_7}$	m
Henry's law	$H^c = 0.2$	-
coefficients	$H^r = 0.02$	-
removal efficiency	$R = (\overline{C}^\iota - C_E^\iota)/\overline{C}^\iota$ for $\overline{C}^\iota > C_E^\iota$	-
design influent concentration	$\overline{C}^\iota = 0.01 C_s^\iota$	kg/m^3
target effluent	$C_E^c = 5 \times 10^{-6}$	kg/m^3
concentration	$C_E^r = 5 \times 10^{-5}$	kg/m^3
air stripping tower	$b_3 = 100$	$m/[(m^3/s)^{b_4} \ (kg/m^3)^{b_6})]$
height coefficients [1]	$b_4 = -0.8$	-
	$b_5 = 0.75$	-
	$b_6 = 1.2$	-
	$b_7 = 0.33$	-

*cost coefficients have been updated to 2002 basis

Table 8
Constraints

Constraint	Description	Equation	Values	Units
1	min. total extraction, Q^{Tmin}	(39)	- 6.4×10^{-2}	m^3/s
2	max. extraction per well, Q^{emax}	(40)	- 6.4×10^{-3}	m^3/s
3	max. injection per well, Q^{imax}	(40)	6.4×10^{-3}	m^3/s
4	Model 1 min. head*, h^{min}	(41)	40	m
	Model 2 min. head*, h^{min}	(41)	10	m
5	max. solute concentration, F_{sw}	(42)	2.0×10^{-2}	-
6	max. total extraction, Q^{Tmax}	(43)	- 6.4×10^{-2}	m^3/s
7	max. head*, h^{max}	(41)	z_{gs}	m
8	HC	(**)	**	-
9	PAT goal, M	(44)	0.05	-
10	PAT time, t_f	NA	3.15×10^8	s

*Note: head datum is bottom of aquifer ($z = 0$ m)

**Note: capture constraint is specified by initial plume configuration

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