Three-dimensional plume source reconstruction using minimum relative entropy inversion

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Received 15 April 1997; accepted 10 November 1997

Abstract

In this paper we extend the minimum relative entropy (MRE) method to recover the source-release history of a three dimensional plume. This extension is carried out in an analytic framework, and in order to qualify as a linear inverse problem the various transport parameters such as dispersivity and the like are considered to be known. In addition, the groundwater flow system is assumed to be steady and uniform. The contributions of this paper include an explanation how MRE can be used as a measure of resolution in linear inversion, a reporting of a three dimensional analytic solution for mass transport in a steady one dimensional velocity field for a variable in-time source loading, an estimation the source-release history for synthetically generated data sets, and an application of the methodology to a case-study problem at the Gloucester Landfill in Ontario, Canada. We found that the relative entropy measure is useful in indicating the reduction in uncertainty between the posterior and prior pdfs as a result of the new information provided by the physical constraints and data. Using the individual model-parameter relative entropies as a measure of resolution, one can make quantitative judgments about which part of the history is likely to be well resolved. Comparing inversion results for synthetic aquifers with one well and two sample points with only one sample point indicates that temporal data at several wells allows for a superior reconstruction of the release history. We investigate the potential benefits of locating sample points on an spatial rather than temporal basis. Results show that early part of the release history is poorly recovered. Comparing these results with one well and two sample points indicates that temporal data at a few wells allows for a better reconstruction of the release history. An incomplete time record is also investigated. Results show that early part
of the release history prior to the commencement of measurements is poorly recovered. It is essential that as much as possible of the time histories of plumes be monitored if the entire release history is to be determined. The MRE approach is used to reconstruct the release history of a 1,4-dioxane plume measured at the Gloucester Landfill in Ontario, Canada. The recovered release history is fairly narrow and generally flat in shape, although two peaks are evident. Neither peak is particularly well defined, judging from the resolution curve and analysis of the confidence ranges. One of the peaks coincides with year 1979, close to the year 1978 in which a large spill was noted. However, a considerable variation of possible source releases is possible. © 1998 Elsevier Science B.V. All rights reserved.

Keywords: Groundwater analysis; Minimum relative entropy; Three-dimensional plume

1. Introduction

A challenging issue in groundwater analysis is the recovery of the release history of a groundwater contaminant source. The study of plume-source histories is particularly relevant for those groundwater professionals who are in the business of trying to partition responsibility of contamination to various parties, or for internal auditing procedures. This particular issue (if the groundwater velocity field and dispersion coefficients are known) can be categorized as a linear inverse problem. Various researchers are engaged in finding new approaches to the more general non-linear inverse problems encountered in groundwater hydrology. The study of linear inversion and resolution provides an important framework for those studies.

Wagner (1992) and Skaggs and Kabala (1994, 1995) present various solutions to the plume-source reconstruction problem and the reader is referred to either of these works for a review. Basically, Wagner (1992) solves an optimization problem for both the contaminant source history and relevant aquifer parameters. Skaggs and Kabala (1994) emphasize the fundamental ill-posed nature of the problem and show how Tikhonov regularization can be used to solve for the source-release history of a one-dimensional groundwater contaminant. These same authors (Skaggs and Kabala, 1995) develop an algorithm based on the concept of quasi-reversibility and obtain another approximate solution. Woodbury and Ulrych (1996) have developed an inference solution which is based on minimum relative entropy (MRE) theory and is described below. Woodbury and Ulrych (1993), Woodbury et al. (1995) and Woodbury and Ulrych (1996) have also applied the MRE principle to the determination of uncertainty in groundwater flow models. The importance of these latter works work lies in the emphasis on the probabilistic approach, which considers parameters to be random variables rather than fixed deterministic quantities. The major stumbling block to the use of probabilistic models is how to assess the statistical properties of unknown model parameters, considering that there is a large degree of uncertainty in their measured values. The MRE approach assigns probability distributions to model parameters in a manner consistent with the principle of maximum entropy, which takes into account known information and is maximally uncommitted with respect to unknown information. Whereas probabilistic studies usually assume Gaussian distributions, the MRE approach assigns truncated exponential distributions where only the lower and upper bounds and
some knowledge of the mean are given. This is very important because we have found that the Gaussian a priori assumption in groundwater related problems is generally too constrictive and injects more information into the solution than is present in the data themselves.

In a particular study, Woodbury and Ulrych (1993) applied the MRE approach to the analysis of the observed spread of a large tracer experiment in Borden Ontario. They compared two types of models, one using volumetric averaging and the other using a stochastic model for the hydraulic conductivity. Results are similar for both models in a probabilistic framework, however the MRE approach allowed a superior reconstruction of the associated pdf.

Woodbury et al. (1995) and Woodbury (1997) also used MRE to establish a priori pdf’s in groundwater analysis where little or no information is available and thereby extended this approach in a rational way to these kinds of problems. We believe these are significant contributions to the probabilistic approach in that virtually any kind of model which involves natural geologic materials may be examined.

As mentioned earlier, Woodbury and Ulrych (1996) show how MRE can be used to formulate a general solution to the linear inverse problem and show how the method can be applied to recovering the release history of a groundwater contaminant in a one dimensional system. In their analysis of a synthetic source-release function developed by Skaggs and Kabala (1994), they found that for noise-free data the reconstructed plume evolution history is indistinguishable from the true history. In comparing their results to SK they found good agreement. The reader is referred to the comment and reply of Kabala and Skaggs (1998) and Woodbury and Ulrych (1998) for detailed discussions of regularization and the MRE approach.

Once a plume source history has been developed, future behavior of a plume can be estimated. One advantage of the MRE approach to inversion is that the plume source is characterized by a probability density function. This function can be sampled randomly and then future predictions can be cast in a probabilistic framework. For an example simulation, the MRE approach was not only able to resolve the source function from noisy data but was also able to correctly predict future behavior.

1.1. Specific new goals

Currently, Woodbury and Ulrych (1996) have solved the one dimensional contaminant-source reconstruction problem with MRE. Their formulation allows for lower and upper bounds and a prior estimate of the mean value of multiple parameters. While that solution is useful from the point of view of demonstrating theory it may have limited practical application. In order to extend the general practicality of the method, we adapt the approach to recover the source-release history of a three dimensional plume. This extension is carried out in an analytic framework, and in this work we report a three dimensional analytic solution developed by Mayer (1992) for mass transport in a steady one-dimensional velocity field for a variable in-time source loading. In order to qualify as a linear inverse problem the various transport parameters such as dispersivity and the like are considered to be known. In addition, the groundwater flow system is assumed to be steady and uniform. It will be shown that the method works well in recovering
release histories of fictitious groundwater contaminant plumes and in that light may prove to be useful in problems where a simplified conceptual model of a site is adopted. The authors consider that a practical application to a case history would also be of benefit in determining if the method could be used in a typical consulting or regulatory environment when the above conditions are not strictly satisfied. For this reason we apply the technique to recovering the release history of a case-study landfill in Gloucester, Ontario. In summary, the major contributions of this paper are:

- An explanation how MRE can be used as a measure of resolution in linear inversion. This is a significant new finding, not explored in any previous work.
- Estimation the source-release history for synthetically generated data sets. We will examine the benefits of using temporal data (i.e., wells monitored over time) and/or spatial data (dense or sparse sampling in three dimensional space).
- Application of the methodology to a case-study problem at the Gloucester Landfill in Ontario, Canada.

2. Minimum relative entropy inversion

Consider the discrete linear inverse problem of the form

\[ \mathbf{d} = \mathbf{Gm} \]  

(1)

where \( \mathbf{d} \) is a discrete set of measured data at \( M \) measurement points, \( \mathbf{G} \) are known kernel functions of the form \( g_{jn} \), and \( \mathbf{m} \) is a set of \( N \) model parameters. We consider ill-posed problems where \( M \leq N \). It is the goal of the inversion to obtain an estimate \( \hat{\mathbf{m}} \) of \( \mathbf{m} \) which satisfies Eq. (1). The model parameter estimation problem is approached from the point of view of probability theory. As Mohammad-Djafari and Demoment (1989) note

Assigning a probability to a parameter value does not mean forcibly that this parameter is a random variable or that the probability is a limit to its realization frequency. The probability is just a measure of our confidence to that value of parameter.

Consider a prior probability density function (pdf) for the model parameters \( p(\mathbf{m}) \) which is based on the upper bound, lower bound, and estimate of the mean value of each parameter. The MRE principle can be used to ‘update’ the prior pdf based on newly considered information of the form Eq. (1) to obtain a posterior pdf, \( q(\mathbf{m}) \). Woodbury and Ulrych (1996) show that the posterior pdf determined by minimization of the relative entropy measure is

\[ q(\mathbf{m}) = p(\mathbf{m}) \exp \left[ -1 - \mu - \sum_{j=1}^{M} \lambda_j \sum_{n=1}^{N} g_{jn} m_n \right] \]  

(2)

The \( \beta \) terms must be determined from the prior information and the \( \lambda \) terms are found by satisfying the expected value constraints Eq. (1) (see Woodbury and Ulrych, 1993).
Defining
\[ a_n = \beta_n + \sum_{j=1}^{M} \lambda_j g_{jn} \]

Woodbury and Ulrych (1996), obtain
\[ q(m) = \prod_{n=1}^{N} \frac{a_n}{\exp(-a_n U) - 1} \exp[-m_n a_n] \tag{3} \]
which is a multivariate truncated-exponential pdf. The estimate \( \hat{m} \) is the expected value of Eq. (2) and performing the integration, Woodbury and Ulrych (1996) obtain
\[ \hat{m}_n = \frac{\exp(-a_n U) a_n U + \exp(-a_n U) - 1}{a_n (\exp(-a_n U) - 1)} \tag{4} \]

Woodbury and Ulrych (1996, 1998) also deal with confidence (credibility) intervals, the treatment of noise and other issues and the reader is referred to those works for details. In such an intervals as stated by Press (1989), we are referring to the probability of a parameter being in an interval that is conditional on the observed data in the current experiment.

2.1. Resolution enhancement

Model resolution is an important aspect of any inverse problem (Parker, 1994). A model resolution matrix (Menke, 1984 pp. 63–64) can be defined that is a function of the data kernel. This matrix characterizes how well an inverse can separate or identify physically adjacent model parameters. Suppose we have an estimate of the model \( m_{est} \) that is computed from some generalized inverse
\[ m_{est} = G^{-\frac{1}{2}} d_{obs} \]
In the above, the inverse of the kernel is written as a means of identifying a ‘generalized’ inverse whose actual form depends on the problem being solved. For a noise-free underdetermined problem with no prior information, this matrix would be \( G^{T} (GG^{T})^{-1} \). Suppose there exists a true solution \( m_{true} \) to an inverse problem, then
\[ m_{est} = G^{-\frac{1}{2}} [Gm_{true}] = Rm_{true} \tag{5} \]
The matrix \( R \) is called the model resolution matrix. If \( R = I \), then each model parameter is uniquely determined. Note that if off-diagonal terms in this matrix exist, then to some degree the model parameters determined in \( m_{est} \) are really weighted averages of the true values. Maximizing resolution, or achieving a ‘delta-like’ resolution matrix, is the goal of the classic Backus–Gilbert inverse method (Backus and Gilbert, 1967, 1968; Menke, 1984). Notice that in Eq. (5), the data are assumed to be noise-free and no prior information on the model parameters has been given.

It can be shown that for a probabilistic-linear inversion, with Gaussian priors and noise, the Bayes’ maximum a posterior solution (MAP) is (Tarantola, 1987 p. 73):
\[ m_{est} = s + \left[ G^{T} C_{d}^{-1} G + C_{p}^{-1} \right]^{-1} G^{T} C_{d}^{-1} (d^{*} - G s) \tag{6} \]
where $s$ is the prior expected value of the parameters and $d^\prime$ are the observed-noisy data with covariance $C_d$. $C_p$ is the prior covariance matrix of the model parameters. Subtracting $s$ from the above yields

$$m^{est} - s = \left[ G^T C_d^{-1} G + C_p^{-1} \right]^{-1} G^T C_d^{-1} G (m^{true} - s)$$

$$= R [m^{true} - s]$$

Which can be expressed in the same form as Eq. (5) provided that the prior model $s = 0$. It can be shown that in the above (Tarantola, 1987 p. 200):

$$R = I - C_q C_p^{-1}$$

In the above $C_q$ is defined as

$$C_q = \left[ G^T C_d^{-1} G + C_p^{-1} \right]^{-1}$$

Notice that if the posterior covariance of $m$, $C_q$, is zero then $R = I$ and perfect resolution exists, regardless of the prior. Note also in Eq. (7) that as prior information is introduced the resolution matrix become a relative measure. In other words, resolution can be seen as (Tarantola, 1987 p. 63):

First, a parameter is well resolved by the data set if its posterior error bar is much smaller than the prior one. More generally, if its posterior marginal probability density is significantly different from the prior one. If, for example, the prior and posterior densities are identical, the parameter is completely unresolved.

Unfortunately for non-Gaussian distributions one cannot write the linear inverse in the form of Eq. (5) and obtain a closed form expression for $R$. In this paper we propose to use marginal-model relative entropies (RE) as a measure of model resolution. Relative entropy is a measure of a directed ‘distance’ in probability space and is suitable for the purpose of examining resolution enhancement. If a prior distribution is uniform or ‘flat’ over a range it has maximum entropy over all other pdfs. If the posterior pdf is a delta function (i.e., probability of one), it has an entropy of zero. The relative entropy between the prior and posterior pdfs is a positive measure that is related to the variance of the posterior pdf and the difference in the prior and posterior means. A sharply peaked posterior pdf (near zero entropy) indicates that the model parameters in question are uniquely determined. It is important to remember that with respect to probabilistic solutions, resolution takes the form of relative terms, and therefore has a different interpretation than the simple form of Eq. (5). Recall that Eq. (5) refers to the ability to separate adjacent model parameters.

We will investigate the connection between resolution and relative entropy for the Gaussian case. It is well known (Menke, 1984) that the posterior pdf from a linear inverse with Gaussian priors and noise is also Gaussian. Defining a prior pdf for a general random vector $x$ as

$$p(x) = \frac{1}{(2\pi)^{n/2}|C_p|^{1/2}} \exp \left[ -\frac{1}{2} (x - s)^T C_p^{-1} (x - s) \right]$$

(8)
and the posterior as:

\[
q(x) = \frac{1}{(2\pi)^{n/2}|C_p|^{1/2}}\exp\left[-\frac{1}{2}(x-\mu)^T C_p^{-1}(x-\mu)\right]
\]  

(9)

then the relative entropy measure Eq. (3) can be written as:

\[
H = \int q(x) \ln\left[q(x)\right] dx - \int q(x) \ln\left[p(x)\right] dx
\]  

(10)

Substituting Eqs. (8) and (9) into Eq. (10) results in (see also Tarantola, 1987 p. 153):

\[
H = \ln \left(\frac{|C_q|^{1/2}}{|C_p|^{1/2}}\right) + \frac{1}{2} \text{Trace} (C_q C_p^{-1} - I) + \frac{1}{2} (\mu - s)^T C_p^{-1} (\mu - s)
\]

or

\[
H = \ln \left(\frac{|C_q|^{1/2}}{|C_p|^{1/2}}\right) - \frac{1}{2} \text{Trace} (R) + \frac{1}{2} (\mu - s)^T C_p^{-1} (\mu - s)
\]

Note that if the posterior mean \( \mu \) is equal to the prior mean \( s \) and if \( C_q = C_p \) then the relative entropy, \( H = 0 \). If the prior and posterior pdfs are uncorrelated Gaussian, the marginal entropy for an individual parameter \( k \) is:

\[
2H_k = 2\ln \left(\frac{\sigma_{q,k}}{\sigma_{k,p}}\right) + \frac{\sigma_{k,q}^2}{\sigma_{k,p}^2} - 1 + \frac{(\mu_k - s_k)^2}{\sigma_{k,p}^2}
\]

or, solving for \( R_k \)

\[
R_k = 2\ln \left(\frac{\sigma_{k,q}}{\sigma_{k,p}}\right) + \frac{(\mu_k - s_k)^2}{\sigma_{k,p}^2} - 2H_k
\]

In the above one can clearly see the connection between relative entropy and model resolution for this uncorrelated Gaussian case.

For the inverse solution presented in this paper, the posterior pdf Eq. (3) is exponential in form and the various model parameters are independent. Therefore, the marginal pdfs of the posterior can be written as

\[
q(m_k) = \frac{-a_k}{\exp(-a_k U) - 1} \exp(-a_k m_k)
\]

Carrying out a similar exercise as for the Gaussian case above yields individual relative entropies:

\[
H_k = \ln \left[\frac{-a_k/\exp(-a_k U) - 1}{-\beta_k/\exp(-\beta_k U) - 1}\right] - \hat{m}_k \sum \lambda_j g_{jm}
\]

(11)

In subsequent analyses this expression will be evaluated and plotted along with recovered model parameters.
Fig. 1. Schematic description of the three dimensional aquifer system. The rectangular patch source is indicated by the hatched area [Mayer and Sudicky, personal communication], see also Table 1.

2.2. Three dimensional plume solution

A convolution representation of a plume’s spatial distribution in three-dimensions is given by Mayer (1992) and the essence of his results is repeated below. The reader is referred to Mayer (1992) for additional details of the derivation and verification of the model. Consider three-dimensional contaminant transport in porous media with steady, uniform groundwater flow. The porous media is semi-infinite in the longitudinal direction \(0 \leq x \leq \infty\), infinite in the horizontal–transverse direction \((-\infty \leq y \leq \infty\), and finite in the vertical direction \(0 \leq z \leq B\). A rectangular first-type patch source is located on the upstream boundary. The system is illustrated schematically in Fig. 1. Solute transport is described by the volumetrically-averaged advection-dispersion equation

\[
\frac{\partial c}{\partial t} + V' \frac{\partial c}{\partial x} - D_{x} \frac{\partial^2 c}{\partial x^2} - D_{y} \frac{\partial^2 c}{\partial y^2} - D_{z} \frac{\partial^2 c}{\partial z^2} + \tau c = 0
\]  

(12)

With \(V' = V_x\), \(D' = D_x/R\), \(D'_y = D_y/R\), and \(D'_z = D_z/R\). Note that \(c\) is the concentration, \(V_x\) is the groundwater velocity, \(D_x\), \(D_y\), \(D_z\) are components of the dispersion tensor, \(R\) is the retardation factor (solid-phase surface reactions are described by a linear equilibrium isotherm) and \(\tau\) is a first order biochemical decay constant (see Domenico and Schwartz, 1990 for more details). Initial and boundary conditions are given by

\[
c(x, y, z, 0) = 0
\]  

(13)

\[
c(0, -y_0 \leq y \leq +y_0, z_2 \leq z \leq z_1, t) = c_0(t)
\]  

(14)

\[
c(\infty, y, z, t) = 0
\]  

(15)

\[
c(x, \pm \infty, z, t) = 0
\]  

(16)

\[
\frac{\partial c}{\partial z}(x, y, B, t) = 0
\]  

(17)
The analytical solution to Eq. (12) subject to Eqs. (13)–(17) is obtained using integral transform techniques and is:

\[
c(x, y, z, t) = \frac{x(z_2 - z_1)}{4B(\pi D'_s)^{1/2}} \int_0^t c_0(\eta) \frac{1}{(t-\eta)^{1.5}} \exp \left[ \frac{(x - V'(t-\eta))^2}{4D'_s(t-\eta)} \right] \\
- \tau(t-\eta) \left[ \text{erfc} \left( \frac{y - y_0}{2(D'_s(t-\eta))^{1/2}} \right) - \text{erfc} \left( \frac{y + y_0}{2(D'_s(t-\eta))^{1/2}} \right) \right] \\
\times d\eta + \frac{x}{(4D'_s)^{1/2} \pi^{1.5}} \int_0^t c_0(\eta) \frac{1}{(t-\eta)^{1.5}} \exp \left[ \frac{(x - V'(t-\eta))^2}{4D'_s(t-\eta)} \right] \\
- \tau(t-\eta) \left[ \text{erfc} \left( \frac{y - y_0}{2(D'_s(t-\eta))^{1/2}} \right) - \text{erfc} \left( \frac{y + y_0}{2(D'_s(t-\eta))^{1/2}} \right) \right] \\
\times \sum_{n=1}^\infty \frac{1}{n} \left[ \sin \left( \frac{n \pi z_2}{B} \right) - \sin \left( \frac{n \pi z_1}{B} \right) \right] \cos \left( \frac{n \pi z}{B} \right) \\
\times \exp \left[ \frac{n^2 \pi^2 D'_s(t-\eta)}{B^2} \right] d\eta
\] (18)

Because \( c_0(t) \) is not given in functional form, it is necessary to divide the input source concentration into a series of discrete steps with constant average concentrations across each step. The resulting term concerning the source concentration can then be taken outside the integral and Gauss–Legendre quadrature is applicable for integration. This leads to the final solution:

\[
c(x, y, z, t_m) = \frac{x(z_2 - z_1)}{4B(\pi D'_s)^{1/2}} \sum_{i=1}^m \Delta c_0(t_i) \int_{t_{i-1}}^{t_m} \frac{1}{(t_m - \eta)^{1.5}} \\
\times \exp \left[ \frac{(x - V'(t_m - \eta))^2}{4D'_s(t_m - \eta)} \right] - \tau(t_m - \eta) \\
\times \left[ \text{erfc} \left( \frac{y - y_0}{2(D'_s(t_m - \eta))^{1/2}} \right) - \text{erfc} \left( \frac{y + y_0}{2(D'_s(t_m - \eta))^{1/2}} \right) \right] d\eta \\
+ \frac{x}{(4D'_s)^{1/2} \pi^{1.5}} \Delta c_0(t_i) \int_{t_{i-1}}^{t_m} \frac{1}{(t_m - \eta)^{1.5}} \\
\times \exp \left[ \frac{(x - V'(t_m - \eta))^2}{4D'_s(t_m - \eta)} \right] - \tau(t_m - \eta)
\]
\[ \times \left[ \operatorname{erfc} \left( \frac{y - y_0}{2(D_y(t_m - \eta))^{1/2}} \right) - \operatorname{erfc} \left( \frac{y + y_0}{2(D_y(t_0 - \eta))^{1/2}} \right) \right] \]
\[ \times \sum_{n=1}^{\infty} \frac{1}{n} \left[ \sin \left( \frac{n\pi z_2}{B} \right) - \sin \left( \frac{n\pi z_1}{B} \right) \right] \cos \left( \frac{n\pi z_1}{B} \right) \]
\[ \times \exp \left[ \frac{n^2\pi^2 D_y(t_m - \eta)}{B^2} \right] d\eta \]  

(19)

The solution is only valid for \( x > 0 \) and \( t_0 > 0 \) and recall that the initial concentrations in the flow field are \( c(x, y, z, 0) = 0 \). See Fig. 2 for a depiction of the time discretization of an input source.

The digital equivalent to Eq. (19) is:

\[ d_j = \sum_{n=1}^{N} g_{jn} m_n \]  

(20)

where \( j = 1 \ldots M \) data points, \( m_n \) is the recovered release history at \( N \) time periods (namely \( C_m(t) \)), \( g_{jn} \) are the kernel functions and \( d_j \) refers to the predicted \( c(x, y, z, t) \).

The inverse problem is to recover the \( m_n \) values from noisy observations of \( d_j \).

3. Recovering the source release history of a 3D plume

In this paper the release history is recovered by using the MRE inverse approach discussed earlier; namely we solve for the posterior pdf \( p[C_m(t)] \), expected values \( \hat{C}_m(t) \), and the cumulative distribution function \( P[C_m(t)] \). These are Eqs. (3) and (4), and Woodbury and Ulrych (1996), Eq. (13).

![Fig. 2. Average source concentrations and differences of average source concentrations.](image)
3.1. Examples with exact data

In the first example we repeat the analysis of Skaggs and Kabala (1994) who used their Equation 25 to generate a synthetic release history. This particular source-loading function is shown on Fig. 3 and is designed to show the recovery of both coarse and fine detail, and is considered to be a difficult inversion problem. Eq. (19) is then used to calculate the ‘true’ data. Fig. 1 shows a sketch of the hypothetical aquifer under consideration. The various parameters are listed in Table 1.

In subsequent simulations we have set $\tau$, the first order decay constant to be zero and $R$, the retardation coefficient to be one. Retardation simply scales the velocity term and since this term is assumed known in this exercise, the inclusion of this effect would likely not produce a significant difference in the results presented in this paper. Inclusion of a decay term would serve to attenuate the contaminant mass and hence affect the kernel functions ability to resolve the parameters. Again, it is considered that inclusion of this effect would not affect the general conclusions presented in this paper, but we hope verify this conjecture in a subsequent application to additional experimental data.

Fig. 4 shows the resulting spatial plume at 100 and 200 days. Figs. 5 and 6 show synoptic sampling of the plume from 0 to 360 days in 10 days increments at various locations within the aquifer. Fig. 5 shows fictitious sample points at $(40,0,0)$ [$x$, $y$, $z$ coordinates], and at $(40,5,0)$. Fig. 6 shows the measured concentration with time at

![Fig. 3. Plume source-release history of Skaggs and Kabala (1994).](image-url)
Table 1
Aquifer parameters

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_r$ (m/day)</td>
<td>1.0</td>
</tr>
<tr>
<td>$a_x$ (m)</td>
<td>1.0</td>
</tr>
<tr>
<td>$a_y$ (m)</td>
<td>0.1</td>
</tr>
<tr>
<td>$a_z$ (m)</td>
<td>0.1</td>
</tr>
<tr>
<td>$D_m^c$ (m²/day)</td>
<td>0.0</td>
</tr>
<tr>
<td>$R$</td>
<td>1.0</td>
</tr>
<tr>
<td>$\tau$ (1/day)</td>
<td>0.0</td>
</tr>
<tr>
<td>Aquifer Depth (m)</td>
<td>3.0</td>
</tr>
<tr>
<td>Source Width (m)</td>
<td>10.0</td>
</tr>
<tr>
<td>Source elevations (m)</td>
<td>0.5–2.5</td>
</tr>
</tbody>
</table>

(80,5,0) and (80,10,0). For the first simulation, 36 points in time are sampled from 0 to 360 days at (40,0,0). The data are perfectly sampled and have no error. The recovered plume release history is shown on Fig. 7 as a bold line. A total of 360 unknowns are determined. The ‘true’ source release history is shown as a light dotted line. The prior model for this case is a constant concentration from 0 to 360 days. Note that this prior is effectively non-informative and could be considered to be geologically ‘smooth’ in some

Fig. 4. Groundwater contamination plume at (a) 100 and (b) 200 days. Plume generated with parameters listed in Table 1 and the Skaggs and Kabala (1994) source function.
sense. In this time period, the prior is set at 0.5 with a lower bound of 0.0 and an upper bound of 1.1. The reconstructed plume evolution history, based on the recovered $\hat{C}_n(t)$, is in good agreement with the true history. The exception to this statement is the obvious ‘jump’ at time equals 350 days. Here, the inversion simply reflects that the contamination generated at the source has not had the time to travel the distance to the observation points. Therefore the kernel functions have no resolving power at later times and MRE simply defaults to the prior expected value. Fig. 8 (dashed line) shows the same recovered plume history along with the relative entropies for each model parameter (Eq. (11)). The RE measure effectively indicates if there has been any reduction in uncertainty between the posterior and prior as a result of the new information provided by the physical constraints and data. Although the posterior mean values closely match the true solution, resolution is ‘poor’ for the two peaks in the source. The RE measure indicates that the concentrations at early and late times, and the trough in the source at 170 days are better resolved than the peaks.

3.2. Examples with measurement errors

A single set of normally distributed random deviates $N[0,1]$ is generated and added to the concentration data according to

$$C^*(x_n,t) = C(x_n,t) + \epsilon \delta_n$$

(21)
Fig. 6. Contaminant concentrations measured at (80,5,0) [stars] and (80,10,0) [crosses].

Here $C(x_n,t)$ is an exact datum, $\delta_n$ is the $n$'th random deviate and $\epsilon$ is the standard deviation of the noise. In the following simulations we use an approach as outlined in Woodbury and Ulrych (1996) and Johnson and Shore (1984) for the modification of MRE for uncertain data. In the following examples $\epsilon$ is set to 0.01 which we can consider to be ‘moderate’ in terms of noise corruption.

The first example with this noise level is shown on Fig. 9. Here the data are sampled at a regular time interval of 10 days at (80,0,0.5). A constant-concentration prior is assumed and an inversion is sought for 360 unknowns. Fig. 9 shows the results and the MRE solution appears to be close to the exact data case but recovers three peaks in the recovered plume history. Note though, that the RE plot (long dashes) indicates that the middle peak is not as well determined as the immediate troughs. We show later that with the inclusion of more data from another well, the middle peak disappears.

Fig. 10 shows the effect of sampling data off the edge of the plume at (80,10,0.5). Note that the MRE inverse basically reproduces the prior distribution and the RE is zero, indicating poor resolution. In this area, the kernel $G$ has no resolving power. Since we have defaulted back to the prior, MRE essentially tells us that there is no information contained in the measured data that can be used to update the prior probability. So, what then is the ‘best’ estimate of the model? The best estimate in a mean square sense is still the prior mean. The true model may not be contained within the 95% confidence
Fig. 7. Source release history of synthetic groundwater contaminant plume. Dotted line is the ‘true’ release history, bold line is the recovered release history from the MRE inverse. Dashed line is a uniform prior estimate. Data measured at (40,0,0).

Fig. 8. Source release history of synthetic groundwater contaminant plume. Dotted line is the ‘true’ release history, bold line is the recovered release history from the MRE inverse. Dashed line is the relative entropy measure which is used as a measure of model resolution. Data measured at (40,0,0).
Fig. 9. Observed data sampled and corrupted with noise (standard deviation of 0.01). Light dotted line is the true signal. The long dashes represent the model relative entropy. Data measured at (80,0,0.5).

Fig. 10. Source release history of synthetic groundwater contaminant plume. Data measured at (80,10,0.5).
Fig. 11 shows the effect of adding additional data. Data are sampled synoptically at (80,0,0.5) and (80,0,1). This type of sampling would reflect perhaps one borehole with two sample points installed. Compare Fig. 11 with Fig. 9. Note that the first peak and trough are better defined and the third-nonexistent peak in Fig. 9 disappears.

3.3. Spatial vs. temporal data

In this section the potential benefits of locating sample points on a spatial rather than temporal basis are investigated. This situation could potentially arise if a contamination plume is discovered and then attempts were made to first determine its areal extent and then second, recover the release history. Although some of the conclusions presented below may seem self evident, the results do provide some insight when the Gloucester Landfill data set is examined later.

Fig. 12 shows the groundwater contaminant plume at 250 days, again based on the base-case parameter set in Table 1. Located on the figure are 72 wells at 0.5 m depth all located on one half of the domain, due to the partial symmetry of the plume. One might expect at the outset that the source release history at early times will be poorly recovered
and indeed Fig. 13 illustrates exactly that point. Notice that the early record is poorly recovered but the first ‘real’ trough at 160 days and the latter section past 200 days are reasonably recovered. Comparing these results with Fig. 11 for one well and two sample points indicates that temporal data at a few wells allow for a better reconstruction of the release history, although this conclusion may depend on where the sample points are located and when they are sampled.

![Figure 12: Groundwater contamination plume at 250 days. Plume generated with parameters listed in Table 1 and the Skaggs and Kabala source function. Seventy two wells sampled.](image1)

![Figure 13: Source release history of synthetic groundwater contaminant plume. Data sampled in 72 spatial locations. Bold line is the ‘true’ release history, dotted line is the recovered release history from the MRE inverse. Dashed line is a uniform prior estimate.](image2)
Fig. 14 shows another scenario: that of an incomplete time record. Suppose a plume was detected, but the synoptic sampling did not begin until 220 days. Two wells with a total of four sample points at $(80,0,0.5)$, $(80,0,1)$, $(80,5,0.5)$ and $(80,5,1)$ have recorded data. Fig. 14 shows results reminiscent of Fig. 13; namely poorly recovered early time histories. Using the RE as a measure of resolution though, one can make quantitative judgments about which part of the history is well resolved. It is apparent that as much of the time histories of these plumes should be monitored if the entire release history is to be determined.

If the properties of equation 23 are not known exactly, or if they vary in space or time the method may not work as well, particularly in a practical setting. In this regard, it is useful to apply the technique to a case history contamination source and attempt a release history reconstruction. The reader should note that very few case studies demonstrating plume source recovery are available.

4. Gloucester Landfill site

It should be noted that an active participation in the various exploration programs was not possible by the authors until the late stages of investigation at this site. In addition, the groundwater flow field may not strictly satisfy the conditions required of the model; namely steady-uniform flow with constant dispersion. It must be emphasized that only a
semi-quantitative analysis of the case study area is possible at this time. However, as we hope the reader will agree, we demonstrate the usefulness of the MRE approach in a typical engineering setting.

4.1. Background information

The Gloucester Landfill site is located south of Ottawa in Ontario, Canada adjacent to the Ottawa International Airport. The site is owned by Transport Canada and was leased to the Township of Gloucester in 1957 for use as a municipal waste disposal site. The site served as a municipal waste disposal site from approximately 1957 to 1980. Beginning in 1969 and until 1980, the site also served as a disposal site for federal laboratory, university and hospital hazardous wastes. These wastes were disposed of in a Special Waste Compound measuring approximately 3000 m² in area located along the western edge of the landfill. Wastes disposed of in the Special Waste Compound consisted primarily of organic solvents although other wastes including DDT, arsenic, cyanide, copper sulfate, hydrofluoric acid, metal carbonates and wood preservative solutions appear to have also been disposed of at the site (Jackson et al., 1985). Disposal practices within the Special Waste Compound generally involved the excavation of trenches to depths of four meters or more followed by the placement and subsequent detonation of the wastes in the trenches. Records pertaining to the volumes of waste materials disposed of in the Special Waste Compound as well as the frequency of disposal events were not kept. On one occasion in 1978, approximately 1 ton of organic solvents was reported to have been disposed of within the Special Waste Compound.

The Gloucester Landfill site is situated on top of a complex sequence of glaciofluvial and littoral deposits of Quaternary age. Specifically, the site lies on the eastern flank of a northwest–southeast trending sand and gravel ridge. Five principal stratigraphic units occur beneath the site. These units include (in order of increasing depth below ground surface): (1) an upper unit on average about 6 m in thickness containing a shallow water table aquifer and comprised primarily of fine sands; (2) a confining layer on average 1±2 m in thickness consisting of clayey silts and silts; (3) a unit comprised of interstratified sequences of silts, sands and poorly sorted gravels up to 25 m in thickness; (4) a dense coarse till unit up to 3 m in thickness; (5) and a limestone bedrock unit containing fractures and cavities over at least the upper 7 m (Jackson et al., 1985). A deep confined aquifer occurs beneath the confining layer (2) within the lower three units. On the basis of exploratory bore holes conducted at the site, the confining layer appears to pinch out toward the western end of the site in the area of the Special Waste Compound.

The confined aquifer at the site has been significantly impacted by wastes disposed of in the Special Waste Compound. Contaminants which have been detected in the confined aquifer include 1,4-dioxane, tetrahydrofuran, diethylether, trichloroethylene, 1,1-dichloroethane, benzene, chlorobenzene, 1,1,2-trichlorotrifluoroethane, 1,1,1-trichloroethane, tetrachloroethylene, chloroform and 1,2-dichloroethane. The observed impact of contamination on the confined aquifer suggests that a direct path for migration of contaminants into the confined aquifer is believed to have occurred in the area of the Special Waste Compound. Possible explanations of the deep contamination include the
possible absence (pinching out) of the confining layer in the area of the Special Waste Compound or the penetration of the confining layer (if present) during disposal-related trenching activities. Since some indiscriminate dumping apparently occurred in the Special Waste Compound, it is not known whether deep excavations beyond the depth of the confining layer may have occurred on occasion.

Most of the contamination found in the confined aquifer occurs in the interstratified unit lying above the bedrock and basal till units (unit 3). The hydraulic conductivity of the interstratified unit, based on numerous slug tests and pump tests conducted at the site, averages $1.1 \times 10^{-2}$ cm/s (Jackson et al., 1985). The hydraulic gradient within the confined aquifer at the site is approximately 0.005. On this basis and assuming an average porosity of 0.3, the calculated average groundwater velocity within the confined aquifer is approximately 15 cm/day, and ranges from 1 to 20 cm/day. Contamination originating from the Special Waste Compound has migrated in an easterly direction away from the compound, and the contaminant plume has gradually moved downward in the confined aquifer toward the till and bedrock units. This behavior is likely due to a decreasing hydraulic conductivity trend in the upper aquifer to the east of the site. This trend may be coupled with increased fracturing and therefore increased hydraulic conductivity in the bedrock to the east of the site. Boreholes completed 3 m into bedrock approximately 500 m to the east of the Special Waste Compound have indicated significant surface fracturing. Bedrock at the site rises rapidly to the east and eventually outcrops approximately 1 km beyond the site. The rapidly rising bedrock coupled with the decreasing distance between the bedrock and the confining layer to the east of the site appears to be responsible for artesian conditions noted in wells installed in the confined aquifer in this area of the site. Increasingly strong upward vertical gradients are also encountered 300–400 m to the east of the site. Vertical gradients are not observed over the initial 300–400 m east of the Special Waste Compound.

The contaminant exhibiting the greatest mobility at the site is 1,4-dioxane ($K_{sw} = -0.27$, solubility $1.2 \times 10^6$ mg/l) which has been identified by the United States Environmental Protection Agency (USEPA) as a probable human carcinogen. 1,4-dioxane is highly soluble in water and is reported to be resistant to biodegradation under both aerobic and anaerobic conditions. Because of its properties, 1,4-dioxane effectively serves as a conservative tracer at the site for evaluating groundwater flow.

By Spring of 1994, the 1,4-dioxane plume within the confined aquifer had migrated at least 500 m to the east, away from the Special Waste Compound. Based on the distribution of 1,4-dioxane at the site within the confined aquifer, a relatively large-apparent longitudinal dispersivity appears to be in effect (> 150 m). This is likely due to the time-varying source function and/or significant layered and trending hydraulic conductivity heterogeneities characteristic of the confined aquifer. The horizontal transverse dispersivity and vertical dispersivities within the confined aquifer were previously estimated at 50 m and 10 m, respectively.

A pump and treat system is currently in operation at the site. The pump and treat system consists of 29 extraction wells; 22 in the shallow unconfined aquifer and 7 in the deeper confined aquifer. The pump and treat system draws approximately 250 l/min from the shallow aquifer and approximately 500 l/min from the confined aquifer. The pump and treat system has been in operation since 1992. Extracted groundwater is
treated at the surface with a UV-peroxide process and is subsequently re-injected into the subsurface at a location up-gradient of the site. Specifically, the extracted groundwater enters a treatment plant facility where it is first collected in a 35,000 l holding tank. Water is then drawn from the holding tank and treated with sulfuric acid to reduce the pH. Once treated with acid, the water is directed to a UV oxidation unit where hydrogen peroxide is added and the water is passed through a series of UV lamp chambers. Upon exiting the UV oxidation system, the water is treated with sodium hydroxide to again raise the pH. Once treated with sodium hydroxide, the water is re-injected into the subsurface at one or more of five injection well locations. Injection of groundwater into the subsurface has created a groundwater mound up-gradient of the contaminant plumes, and has affected the hydraulic gradient in both the shallow and deep aquifers. However, the hydraulic gradients do not appear to be affected for more than 100 m beyond the Special Waste Compound.

4.2. Assessment of Parameters

Fig. 15 shows a plan view and contours of three plumes of organic contaminants measured in 1982. Based on an analysis of the center of mass of the plume an estimate of 12.7 cm/day groundwater velocity is calculated. Approximate analysis of the plume moments and comparisons to classic theory (Domenico and Schwartz, 1990) suggest a longitudinal dispersivity of 2.6 m and transverse–horizontal dispersivity of 0.5 m. These values are generally consistent with reported values in the literature. Of course, the determination of the dispersivity itself depends on a constant source loading which is precisely the object of this analysis. Nevertheless, the answers are surprisingly robust with respect to uncertainty in dispersivity (Skaggs and Kabala, 1994). The remainder of the parameters listed on Table 2 are arise from an analysis of the available data (Jackson et al., 1985). We have assumed that the special waste activities commenced in May 1, 1969 which represents time equals zero.

4.3. Source Recovery

Very little is known about the release history of 1,4-dioxane at the site. The exact time operations commenced is approximate, as is the range of concentrations to be expected. The only other information available is that a large spill occurred sometime in 1978. Therefore, we have sought a solution consisting of a lower bound of 0 mg/l, and an upper bound of the solubility of 1,4-dioxane in water. The prior expected value consists of a Gaussian shape centered in 1978 with a range of 600 days and a peak value of 100 mg/l.

The data set consists of measured concentrations in a number of multi-port samplers taken in 1982, and spring/summer 1994, 1995, and 1996. A total of 136 data points are available. Fig. 16 shows the recovered release history and the parameter relative entropy curve. The release history is fairly narrow and flat in shape, although two peaks are evident. Neither peak is particularly well defined, judging from the resolution curve. The
two peaks coincide with times of 8.4 and 9.7 years. The latter time corresponds to mid 1978, in the year in which a large spill was known to occur (see Section 4.2), although this could be fortuitous. Note that the first data set available to us was in 1982 or at time 4745 days. One might expect that a similar situation to the incomplete time record (Fig. 16). Fig. 16. Source release history of 1,4-dioxane recovered from the Gloucester Landfill. Solid line represents the release history and the dashed line the relative entropies for each value of recovered concentration at a particular time. Gaussian prior.
Fig. 17. Source release history of 1,4-dioxane recovered from the Gloucester Landfill. Solid line represents the release history and the dashed line the relative entropies for each value of recovered concentration at a particular time. Uniform prior.

Fig. 18. Source release history of 1,4-dioxane recovered from the Gloucester Landfill. Solid line represents the expected value of the release history and the dashed lines correspond to the upper 95 percentile and lower 5 percentile, respectively.
14) problem presented earlier; namely poor resolution at early times. Interestingly, the highest resolution does correspond to a time of about 3300 days or early 1978.

Fig. 17 shows the recovered release history if one assumed a uniform prior between early 1978 and late 1980, the termination of activities at the Waste Compound. The prior concentration was assumed to be 100 mg/l during this period. The results are generally similar to the previous runs. Peaks are found at 3300, 3850 and 4425 days, although the latter resolution is poor. Note that the standard deviation in the residuals is about 0.15 mg/l which is a small portion of the recovered release history. Fig. 18 shows the upper 95 percentile and the lower 5 percentile confidence ranges. As seen, a considerable variation of possible source releases within that range is possible. The authors believe that the best interpretation obtainable from this modeling exercise suggests that (1) it is not possible to resolve the source release history prior to 3200 days and after about 4400 days, and (2) there is a 90% probability that the ‘true’ source release lies within a range of about 0.1 to 2 mg/l between those two dates. This is a vast improvement on the prior information which had an upper limit of 1.2 × 10^6 mg/l. Depending upon the nature of an assessment, such a determination may be quite adequate.

5. Discussion and conclusions

Previous works by Woodbury and Ulrych (1996) have shown that given prior information in terms of a lower and upper bound, a prior bias, and constraints in terms of measured data, minimum relative entropy (MRE) yields exact expressions for the posterior pdf and the expected value of the linear inverse problem. In this paper we outline how MRE can be used as a measure of resolution in linear inversion, describe a three dimensional analytic solution for mass transport in a steady one dimensional velocity field for a variable in-time source loading, and estimate the source-release history for synthetically generated data sets. We examine the benefits of using temporal data (i.e., wells monitored over time) and/or spatial data (dense or sparse sampling in three dimensional space).

We show how the approach developed in this paper is applied to the problem of recovering the release histories of plumes in a three dimensional, constant velocity and dispersivity systems. We found that:

(1) The relative entropy measure is shown to be very useful in indicating reduction in uncertainty between the posterior and prior as a result of the new information provided by the physical constraints and data. In a series of runs the RE shows directly if the posterior pdf has a lower entropy than the prior. A lower entropy is related to a smaller variance in the posterior pdf.

(2) We use an approach as outlined in Johnson and Shore (1984) for the modification of MRE for uncertain data. In the examples ε is set to 0.01 which we can consider to be ‘moderate’ in terms of noise corruption. Comparing results with one well and two sample points with only one sample point indicates that temporal data at several wells allows for a superior reconstruction of the release history. Since the majority of the cost of obtaining contaminant information relates to drilling costs, this observation suggests that multiple sample points add greatly to the resolution of the inverted source-history.
(3) We investigate the potential benefits of locating sample points on an spatial rather than temporal basis. This situation could arise if a contamination plume is discovered and then attempts are made to determine its areal extent and then use this information recover the release history. Results show that early part of the release history is poorly recovered. Comparing these results with for one well and two sample points indicates that temporal data at a few wells allow for a better reconstruction of the release history.

(4) An incomplete time record was also investigated. Suppose a plume was detected, but the synoptic sampling did not begin until mid-way through the release. Results show that early part of the release history is prior to the commencement of measurements is poorly recovered. Using the RE as a measure of resolution, one can at least make qualitative judgments about which part of the history is likely to be well resolved. It is essential that as much as possible of the time histories of these plumes be monitored if the entire release history is to be determined.

(5) Finally the approach is used to reconstruct the release history of a 1,4-dioxane plume measured at the Gloucester Landfill in Ontario, Canada. It should be noted that an active participation in the various exploration programs was not possible by the authors until the late stages of investigation at this site. In addition, the groundwater flow field may not strictly satisfy the conditions required of the model; namely steady-uniform flow with constant dispersion. It must be emphasized that only a semi-quantitative analysis of the case study area is possible at this time. However, as we hope the reader will agree, we demonstrate the usefulness of the MRE approach in a typical engineering setting. The recovered release history is fairly narrow and flat although two peaks are evident. Neither peak is particularly well defined, judging from the resolution curve and analysis of the confidence ranges. The two peaks coincide with times of 8.4 and 9.7 years. The latter time corresponds to the year 1978, in which a large spill was noted. The highest resolution also corresponds to that time. As shown, a considerable variation of possible source releases is possible. The authors believe that the best interpretation obtainable from this modeling exercise suggests that (1) it is not possible to resolve the source release history prior to 3200 days and after about 4400 days, and (2) there is a 90% probability that the ‘true’ source release lies within a range of about 0.1 to 2 mg/l between those two dates. Depending upon the nature of an assessment, such a determination may be quite adequate.

Acknowledgements

This research was funded by grants from the Natural Sciences and Engineering Research Council of Canada (NSERC). Computations were carried out on computer facilities supported by grants from the University of Manitoba. The analytic solution to the three dimensional rectangular-patch source was developed by Ulrich Mayer for a thesis completed under Ed Sudicky’s direction in 1992, and we acknowledge his contribution. Keni Zhang produced some of the computer code used in this paper and also assisted in preparing data sets from the large volume of material collected from the Gloucester landfill. His assistance is gratefully acknowledged. Thanks are also extended to Zbigniew Kabala for his review of an earlier version of this manuscript.
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