

HYDROLOGIC INVERSION USING MARCHING-JURY BACKWARD BEAM EQUATION AND QUASI-REVERSIBILITY METHODS

Daniel Cornacchiulo¹, Amvrossios C. Bagtzoglou¹, Associate Member ASCE,
and Juliana Atmadja²

ABSTRACT: In this paper, a comparison between the *Marching-Jury Backward Beam Equation (MJBBE)* and the *Quasi-Reversibility (QR)* methods to perform hydrologic inversion and, more specifically, to reconstruct conservative contaminant plume spatial distributions is presented. Spatially uncorrelated and correlated, non-stationary, heterogeneous dispersion coefficient fields were generated using the *Bayesian Nearest Neighbor Method (B-NNM)*. The *MJBBE* is found to be robust enough to handle highly heterogeneous parameters and is able to preserve the salient features of the initial input data. On the other hand, the *QR* method is superior in handling cases with homogeneous parameters and with initial data that are plagued by uncertainty but it performs very poorly in cases with heterogeneous media.

INTRODUCTION

Naturally occurring porous media are highly heterogeneous, and are characterized by spatially variable geometric and hydraulic properties. With increasing demands for clean drinking water and a way to identify pollution sources accurately, it is clear that a method that can backtrack the pollution source in order to perform contaminant plume spatial distribution recovery and ultimately reconstruct the plume release time history in heterogeneous media is highly desirable. For the past fifteen years, several attempts have been made to tackle one of the most difficult problems of hydrologic inversion, namely to solve the Advection Dispersion Equation (ADE) backwards in time in order to identify the pollution source. Even though this topic is of considerable interest, only recently several review papers appeared in the literature. For example, Morrison (2000a) presented an extensive literature review of commonly used environmental forensic methods for age dating and source identification. In this paper, Morrison discussed commonly used environmental forensic techniques and their possible applications so that readers can decide which technique is most appropriate for their cases. A more in-depth review of these techniques can be found in Morrison (2000b). More recently, Atmadja and Bagtzoglou (2001b) presented a state-of-the-art report on mathematical methods that could be used for pollution source identification.

¹Department of Civil Engineering & Engineering Mechanics, Columbia University, New York, NY 10027; E-mail: abagtzog@civil.columbia.edu, dc460@columbia.edu

²TAMS Consultants, Inc., Bloomfield, NJ 07003; E-mail: jatmadja@tamsconsultants.com

SIMULATION OF HETEROGENEITY IN POROUS MEDIA

In this paper we apply the method presented by Bagtzoglou and Ababou (1997) to generate unconditional, spatially correlated Gauss-Markov random fields using the *Bayesian Nearest Neighbor Method (B-NNM)*. A 1D domain of length $L=42$ discretized using a grid of $\Delta x=0.5$ is considered for our test cases. We have used variable dispersion coefficients that account for deviations in the transport velocity caused by variability in porosity. We used different values of $D(x)$ in two different zones. The two zones are: (1) outer zones for $0 \leq x < 11$ and $17 < x \leq 42$; and (2) inner zone for $11 \leq x \leq 17$. The configuration used employs $D_o=1$ for zone 1 and $D_i=8$ for zone 2 and *vice versa*. Spatially uncorrelated heterogeneous media were simulated using a randomly generated, normally distributed, dispersion coefficient with different standard deviation (\mathbf{s}) around the mean value (\mathbf{m}).

For the stationary fields, the mean value of D is one and two different standard deviations ($\mathbf{s}=0.2$ and 0.4) are used for a Coefficient of Variation (CV) of 20 and 40%, respectively. These CV values correspond to upper bounds characteristic of porosity variability in unconsolidated and consolidated media, respectively. For the spatially correlated fields the same mean value and standard deviations used in the case of uncorrelated fields are employed with two different spatial correlation lengths, l of $2 \times \Delta x$ and $4 \times \Delta x$. For the case of spatially correlated, non-stationary fields, D configurations similar to those used with spatially uncorrelated fields but with correlation length of $4 \times \Delta x$ only are used. Within each of the two zones the dispersion coefficient field is stationary. All results presented are based on single realizations and the same field is used for both forward and backward time simulations. In the strict mathematical sense then the dispersion fields used in this work are not random. However, the single realizations of the dispersion coefficient field are completely different from one test case to the next.

In all the analyses, we kept the transport velocity term, u , as constant with a value of one and flow being from the left to the right of the domain. In this work we are dealing with a 1D, steady-state flow problem. Therefore, the only possibility for the transport velocity to be heterogeneous is due to the spatial variability in porosity, which is small and is often ignored. Therefore, the constant velocity represents the mean velocity in the aquifer and the variation in the dispersion coefficient accounts for deviations caused by the variability in porosity.

PLUME RECOVERY IN RANDOMLY HETEROGENEOUS MEDIA

The *Backward Beam Equation (BBE)* was first developed by Carasso (1972). The *BBE* solves parabolic problems backwards in time and can be obtained by differentiating the governing equation of a parabolic equation with respect to time. Let:

$$P = \left(\frac{\partial}{\partial x} \left[D(x) \frac{\partial}{\partial x} \right] - \frac{\partial}{\partial x} [u(x)] - k \right).$$

Using the central difference approximation for the $\frac{\partial^2}{\partial t^2}$, $\frac{\partial^2}{\partial x^2}$ and $\frac{\partial}{\partial x}$ terms and denoting by w^n a vector of w values at all discrete spatial locations at time step n :

$$\frac{(w^{n+1} - 2w^n + w^{n-1}))}{\Delta t^2} - A w^n = 0, \quad n=1, 2, \dots, N_t-1 \quad (1)$$

$$w^{N_t} = e^{kT_{bi}} f_2, \quad w^0 = 0, \quad (2)$$

where N_t is the number of discrete temporal points, $A = P^2$ and the approximation

RESULTS AND DISCUSSION

For all simulations, we ran the forward ADE simulation up to time $t=T_{fi}=2$ and assumed this as our present day configuration. We also saved the forward results at different snapshots in time and treated these as our exact plume distribution for comparison purposes. Using the *MJBBE* and *QR* methods, the concentration configuration at $t=T_{fi}=T_{bi}$ is taken as $f_2(x)$. Since in the *MJBBE* method one needs to assume the spatial distribution of the attribute of interest at $t=0$ to be equal to zero, the spatial distribution at that time will be impossible to recover. Therefore, in our synthetic examples, we assumed our terminal time to be $t=T_{br}=1$ (i.e., the furthest back we can hope to recover is $t=1$) and there is no recoverable concentration distribution for $t<1$. In this case, our total time of simulation becomes $T_{sim}=T_{br}-T_{br}=1$. We want to recover the spatial distribution from $t=2$ to $t=1.1$, which is approximately half of the duration of the forward simulation. For both *MJBBE* and *QR* methods we used $Dx=0.5$ and $Dt=0.02$. The following two error measurements are used as indicators of the *MJBBE* and *QR* performance:

- mass error, normalized by the exact mass, as given by the corresponding forward simulation result,
- concentration peak error, normalized by the exact peak concentration, as given by the corresponding forward simulation result.

Errors of the results were compared at different snapshots backward in time, namely 20% and 90% back in time (t_b) for consistency purposes. However, only the 90% back in time results are presented for the sake of brevity. All results are presented for $x \in [0,30]$ because no concentration changes are detected past $x=30$.

For the *MJBBE* the mass error is only 0.02% (Figure 1) for configuration UN1 (no spatial correlation). Even though the peak error grows about almost ninefold from 0.032% at $t_b=0.2T_{sim}$ to 0.26% at $t_b=0.9T_{sim}$, the error value is still significantly less than 1%. The *QR* method does not perform well in the case of non-stationary heterogeneous fields. In heterogeneous media, the mass conservative nature of the *QR* still holds. The mass error for configuration UN1 increased from -0.02% at $t_b=0.2T_{sim}$ to 0.35% at $t_b=0.9T_{sim}$ (Figure 1). The mass error increase does not seem to be too significant. However, we observed a large concentration fluctuation especially further back in time (Figure 1). Whereas mass errors are increased slightly, the peak errors were increased significantly to -4.72% at $t_b=0.2T_{sim}$ and -56.00% at $t_b=0.9T_{sim}$.

For configuration CN1, where we have a correlation length $I=4Dx$, the *MJBBE* results showed that the correlation length does not have any effect on the *MJBBE* performance. Both mass and peak errors remained the same, with an exception of the peak error at $t_b=0.2T_{sim}$ where the value increased from 0.032% to 0.034% for UN1 and CN1, respectively. Furthermore, the *MJBBE* performance is consistent with the previous results, namely it preserves the shape of the input data. The *QR* method gives the worst peak errors for cases where $m > m_b$ (configuration UN1 and CN1). Similar to the *MJBBE* results, in the case of the *QR* method, the correlation length does not affect the mass errors at $t_b=0.2T_{sim}$. However, the correlation length helps the *QR* method performance further back in time. At $t_b=0.9T_{sim}$, the mass error was improved from 0.35% for UN1 to 0.29% for CN1 (Figure 1 versus 2). The effect of correlation length in the domain is more pronounced for the concentration peak of the recovered plume. The peak errors are better for configuration CN1. We observed an improvement of about 2 to 6% compared to the uncorrelated spatially distributed media. At $t_b=0.2T_{sim}$, the peak error was -3.33% and at $t_b=0.9T_{sim}$, the value was -50.32% (Figure 2).

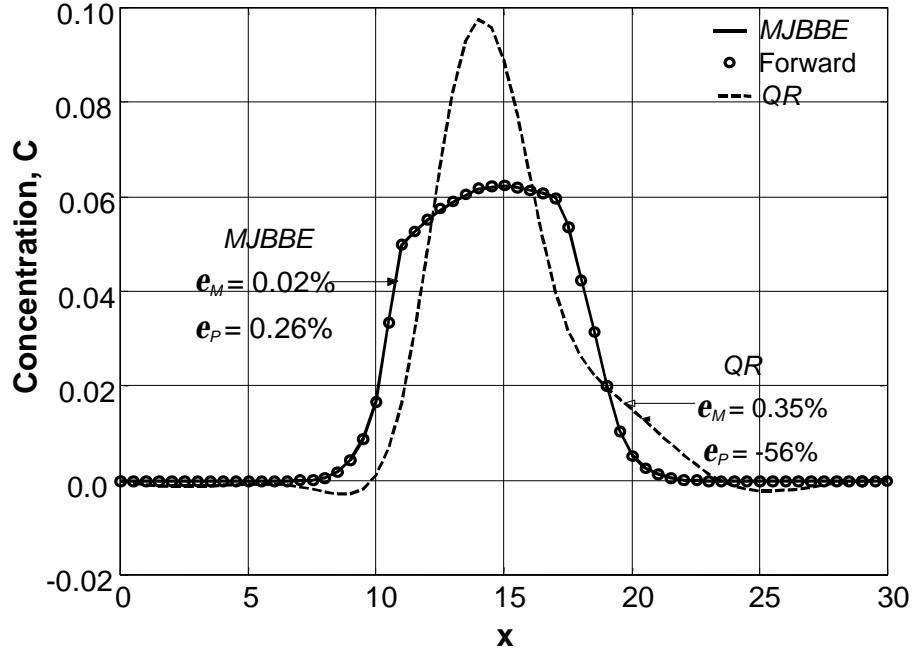


Figure 1. Comparison between *MJBBE* and *QR* methods for non-stationary, spatially uncorrelated heterogeneous medium

In our heterogeneous configuration UN2 where $\mathbf{m}_b > \mathbf{m}$, the *MJBBE* exhibits the worst mass and peak errors. This is consistent with our observation for the deterministically heterogeneous media. The value of the mass error is 0.01% for $t_b = 0.2T_{sim}$ and it grows to 0.06% for $t_b = 0.9T_{sim}$. Adding spatial correlation to the heterogeneous field, which translates into increasing the correlation length from $0Dx$ to $4Dx$ (configuration CN2), improved the performance of the *MJBBE* in terms of the mass error. However, the *MJBBE* generated a worse peak error at $t_b = 0.9T_{sim}$ compared to the uncorrelated field. Unlike the *MJBBE* method, the *QR* method performed better when $\mathbf{m}_b > \mathbf{m}$. At $t_b = 0.2T_{sim}$ the peak errors for the uncorrelated field (UN2) are 0.03% and -4.24% at $t_b = 0.2T_{sim}$ and $t_b = 0.9T_{sim}$, respectively. We were not able to obtain a value for \mathbf{e} that can reconstruct the spatial distribution with a good accuracy. No matter what value of \mathbf{e} we used, we always observed concentration fluctuations, which are more pronounced at later times. For the correlated field, both mass and peak errors are better than that of the uncorrelated one (Table 1). We also observed that the peak concentration recovered by the *QR* method lags compared to the forward simulation, especially at $t_b = 0.9T_{sim}$.

Consistent with the previous observation for configuration CN1, the correlation length helps the performance of the *QR* method in terms of the values of the mass and peak errors. Even though the values of the errors for the *QR* method are improved by adding spatial correlation, the concentration fluctuations are worse. We were able to obtain a peak error of -1.79% at $t_b = 0.9T_{sim}$, but the price to be paid is the increase in the observed negative concentrations. Summary of the errors, optimal k , and \mathbf{e} values for both methods can be found in Table 1.

CONCLUSIONS

We applied the marching jury backward beam equation and the quasi-reversibility methods to recover the non-reactive contaminant spatial distribution in a 1D randomly, non-stationary heterogeneous with and without spatial correlation porous medium. The randomly heterogeneous dispersion field used in this work was generated using the Bayesian Nearest Neighbor Method after Bagtzoglou and Ababou (1997). The *MJBBE* method was able to reconstruct the spatial

distribution of the contaminant plume with very good accuracy. More importantly, the method was able to preserve the shape and salient features of the input data. Conversely, the *QR* method is mass conservative for the homogeneous case but it performed poorly in solving heterogeneous cases. The method introduces concentration fluctuations, especially for configurations where the outer zone has a higher value of dispersion coefficient than the inner zone.

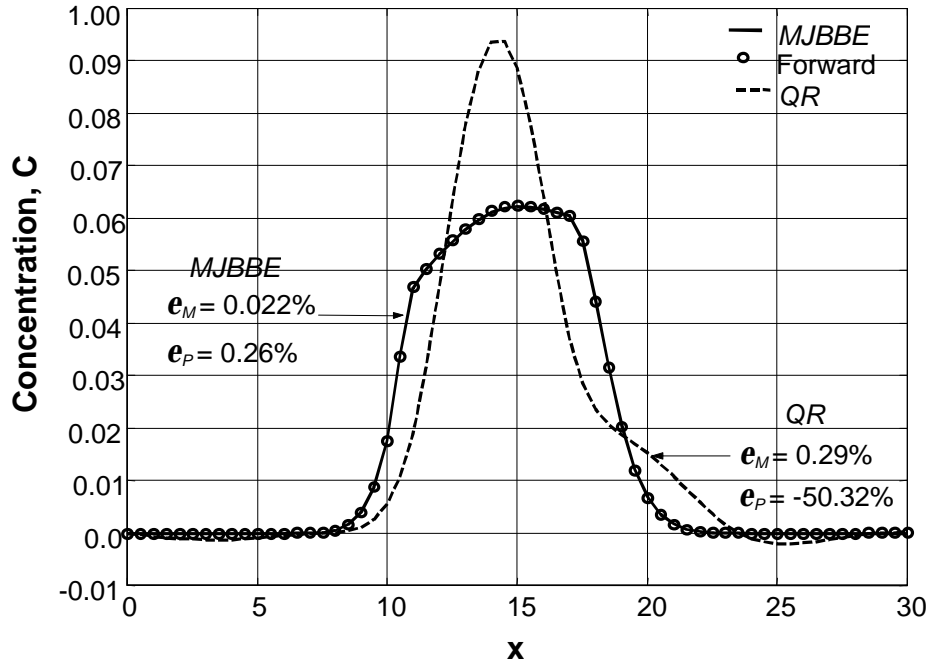


Figure 2. Comparison between *MJBBE* and *QR* methods for non-stationary, spatially correlated heterogeneous medium

For a given value of CV in the dispersion coefficient field, the *MJBBE* performance is the same for spatially uncorrelated and correlated parameters. In addition, in the case of correlated fields, increasing the correlation length did not change the mass error created by the *MJBBE*. On the other hand, when the CV value is increased for a correlated heterogeneous field the *MJBBE* generated slightly larger peak errors further back in time. Adding a small random perturbation to the homogeneous case affected the performance of the *QR* method tremendously, especially in the peak errors. Given the same CV, different correlation lengths did not affect the behavior of the *MJBBE*. However, increasing the value of the CV and correlation length, improved the performance of *MJBBE*. Similar observations can be made for the *QR* method. In addition to smaller mass and peak errors, increased CV and correlation length values improved the *QR* results' phase lag.

For non-stationary heterogeneous media, both *MJBBE* and *QR* perform the worst when the outer zone has a higher dispersion coefficient than the inner zone. The *MJBBE* method created the worst mass errors, while the *QR* method showed negative concentrations and concentration fluctuations. When the dispersion coefficient of the outer zone is lower than the inner zone, the *MJBBE* performed better. As for the *QR* method, it performs poorly for the uncorrelated field by exhibiting concentration fluctuations. Increasing the correlation length of the system did not

improve the fluctuations and the method smoothed out the results acting as if there were no heterogeneity in the field. Suffices to say that, due to this smoothing behavior, the *QR* method is, in general, not capable of preserving the shape of the true plume distribution.

Table 1. Comparison between errors in the *MJBBE* and *QR* methods and required stabilization parameters for various types of heterogeneity

Configuration	<i>MJBBE</i>					<i>QR</i>				
	<i>k</i>	ϵ_M (%)		ϵ_P (%)		<i>e</i>	ϵ_M (%)		ϵ_P (%)	
		$0.2T_{sim}$	$0.9T_{sim}$	$0.2T_{sim}$	$0.9T_{sim}$		$0.2T_{sim}$	$0.9T_{sim}$	$0.2T_{sim}$	$0.9T_{sim}$
UN1	8.7	0.005	0.02	0.032	0.26	8	-0.02	0.35	-4.72	-56.00
UN2	8.7	0.01	0.06	0.08	0.36	10	0.03	-4.24	22.52	36.34
CN1	8.7	0.005	0.02	0.034	0.26	7	-0.02	0.29	-3.33	-50.32
CN2	8.7	0.006	0.03	0.08	0.47	8	0.02	-1.8	19.07	-0.73

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