

## A Combined Probabilistic/Nonprobabilistic Decision Analysis for Contaminant Remediation\*

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**Abstract.** Groundwater contaminant remediation poses a significant challenge due in large part to ubiquitous uncertainties and unknowns. A number of remedial options are typically available at a given contamination site. However, choosing the best option is challenging, because it is not typically known beforehand how effective each remediation will be. Nonetheless, choices must be made. We present an approach to decision support consisting of three coupled layers accounting for model/parametric uncertainties and unknowns. The inner and outer layers employ an information-gap approach to uncertainty quantification, while the middle layer employs Bayes' theorem. Two synthetic remedial scenarios are explored to demonstrate the efficacy of the approach. Considered remedial actions are natural attenuation (NA) and an enhanced attenuation (EA).

**Key words.** decision analysis, Bayesian analysis, information-gap

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**1. Introduction.** There is a pressing need for better tools that empower remedy selection for contaminated groundwater. The U.S. National Research Council recently estimated that the cost to clean up (i.e., remediate) sites that federal law mandates to be remediated is over \$100 billion, with the Department of Energy's burden being approximately \$20 billion [9]. Uncertainty plagues remedy selection. There is often substantial uncertainty in the contamination extent and concentrations, the rate and location at which contamination reaches the aquifer, the rate at which biogeochemical reactions are attenuating or exacerbating the problem, the direction and velocity of the groundwater flow, the rate and type of dispersion, diffusion and pore-scale mixing, large- and small-scale geological features and heterogeneities, and performance and effectiveness of remedial actions. The list could go on, and each of these uncertainties could be further subdivided and expanded. On top of known-unknowns, there are unknown-unknowns. It is therefore not surprising that court mandated remediations fail almost 90% of the time, often due to unforeseen complexities [9].

Scientifically defensible remediation selection requires consideration of all the existing uncertainties and unknowns. See [16] for a review of state-of-the-art approaches to dealing with uncertainty in subsurface hydrology. Probabilistic analyses are frequently performed to under-

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stand the environmental and human-health risks associated with contaminated groundwater sites [15, 3]. Purely probabilistic methods, in comparison to best-estimate or worst-case methods, are a step in the right direction, but the severe uncertainties that are present in subsurface hydrology recall the words of R.A. Fisher in a letter to A.C. Aitken (emphasis ours) [5]:

From this point of view it is almost unfortunate that a group of cases has been found in which inductive inference may properly be expressed in terms of probability, using the fiducial mode of argument; for this has tempted some mathematicians, and will, I fear, tempt more, to imagine that this type of argument is more widely applicable than is really the case, and to avoid enlarging their imaginations sufficiently to grasp *the cases where no probability statement is adequate*.

Bayes' theorem is one of the most popular techniques for probabilistic uncertainty quantification (UQ) (see, e.g., [8, 14, 4]). It is effective in many situations, because it updates our understanding of the uncertainties by conditioning on real data using a mathematically rigorous technique. Bayes' theorem is mathematically rigorous, but its application in science and engineering is not always rigorous. There are two reasons for this:

1. We can enumerate the possible outcomes of dice-rolling but not the possible outcomes of groundwater contamination remediation.
2. We can precisely determine conditional probabilities for coin-tossing, but substantial uncertainty surrounds the conditional probabilities for groundwater contamination remediation.

Of course, Bayes' theorem is rigorously applicable beyond dice-rolling and coin-tossing, but even in cases that are constructed to be simple with ostensibly good probabilistic models, applying Bayes' theorem to the real world may not work as well as one might expect [1]. Bayes' theorem is rigorously applicable only if all possible events can be described, and their conditional probabilities can be derived rigorously. Outside of this domain, it may still be useful, but its use lacks at least some rigor.

To overcome these issues, we employ a three-layered-onion approach. The inner layer employs a nonprobabilistic UQ methodology called "information-gap" [2] to overcome reason 1. The inner layer captures model uncertainty. The middle layer employs Bayes' theorem conditioning on available data. The middle layer captures parametric uncertainty. The outer layer employs another information-gap approach to overcome reason 2. The outer layer captures uncertainty in the conditional probabilities used during the application of Bayes' theorem.

The Bayesian-information-gap approach to UQ is independent of the physical model and implemented in the existing open-source MADS code [17]. This makes it possible to employ the approach on a laptop with simple physical models or a supercomputer with complex physical models.

The remainder of this manuscript is organized as follows. Section 2 contains a description of the framework. Section 3 describes a demonstration of the method to groundwater contaminant remediation scenarios. Section 4 presents a summary and conclusions.

**2. Combining Bayes' theorem with information-gap decision theory.** Suppose that there is a parametric model,  $C(\mathbf{x}, t; \mathbf{P})$ , for predicting the concentrations at location  $\mathbf{x}$  and time  $t$  with uncertainty in the parameters,  $\mathbf{P}$ . The predictive model can be physics or systems based.

The actual concentration is given by the concentration predicted by the model plus or times an unknown error term

$$(1) \quad C(\mathbf{x}, t) = C(\mathbf{x}, t; \mathbf{P}) + E(\mathbf{x}, t; \mathbf{P})$$

or

$$(2) \quad C(\mathbf{x}, t) = C(\mathbf{x}, t; \mathbf{P})E(\mathbf{x}, t; \mathbf{P}).$$

The latter case can be effectively reduced to the former case by taking logarithms and looking at log-concentrations rather than concentrations. We employ the former case, (1), throughout, with the understanding that all of the discussion immediately applies to the latter if log-concentrations are used in place of concentrations. In (1),  $E(\mathbf{x}, t; \mathbf{P})$  represents the error due to improper parameterization and/or inability of the model to reproduce the field concentrations. Frequently, subsurface contaminant concentration measurements have been obtained at a number of monitoring well locations and a number of observation times, and they are used in model calibration to estimate model parameters and/or their probabilistic distribution. Let  $\mathbf{x}_i$ ,  $i = 1, 2, \dots, N_w$ , denote the well locations,  $t_{i,j}$ ,  $j = 1, 2, \dots, N_{t,i}$ , denote the observation times at well  $i$ , and  $\hat{C}(\mathbf{x}_i, t_{i,j})$  denote the measurement at well  $i$  at time  $t_{i,j}$ . The measurement error can be decomposed in a way similar to the model error

$$(3) \quad \hat{C}(\mathbf{x}_i, t_{i,j}) = C(\mathbf{x}_i, t_{i,j}) + \hat{E}(\mathbf{x}_i, t_{i,j}).$$

For the purposes of contaminant remediation, it is very important to know what the concentrations will be or whether the concentration will exceed a threshold,  $C_c$ , at some point,  $\mathbf{x}_c$ , and time,  $t_c$ , in the future (or, more generally, at a collection of points and times;  $C(\mathbf{x}, t) > C_c$ ). This information would also be useful, e.g., for evaluation of the need for remediation or for comparing the cost-effectiveness of alternative remediation scenarios. However, obtaining this information is problematic due to parametric uncertainty and model inadequacy (both captured via  $E(\mathbf{x}_c, t_c; \mathbf{P})$ ). The measurement error ( $\hat{E}(\mathbf{x}_i, t_{i,j})$ ) makes it difficult to determine optimal parameters and the degree of model inadequacy. The uncertainties come from

- measurement errors (e.g., laboratory-analysis errors, deviations from the field sampling procedures, etc.);
- discrepancies between model resolution and sample volumes, akin to forcing a round peg (the measurements) into a square hole (the model computational grid);
- discrepancies between the model's representation of the flow medium properties and the actual aquifer conditions (e.g, upscaling, heterogeneity, anisotropy, etc.); and
- inadequacy of the model (e.g., the model may not represent the actual governing processes accurately and/or precisely).

As a result, the errors may be neither independent nor unbiased.

There are a number of ways for dealing with this uncertainty. One option is to use a single prediction (e.g., best-guess or worst-case) [10]. Using a best-guess prediction essentially ignores the issue of uncertainty. Using a worst-case prediction can be overly pessimistic (if the actual worst-case scenario is used) or optimistic (if the actual worst-case scenario is worse than anticipated). Given that failures in subsurface contaminant remediation are frequently

due to complexities that were not considered [9], it would not be surprising for an ostensibly worst-case prediction to be optimistic.

Another option is the Bayesian approach. The basic Bayesian approach begins by assigning a prior probability distribution to the parameters and then conditioning on the measurements to compute a posterior distribution for the parameters. A conditional distribution for the measurement given the prediction is needed. Combining some algebra with (1) and (3) results in

$$(4) \quad \hat{C}(\mathbf{x}_i, t_{i,j}) = C(\mathbf{x}_i, t_{i,j}; \mathbf{P}) + E(\mathbf{x}_i, t_{i,j}; \mathbf{P}) + \hat{E}(\mathbf{x}_i, t_{i,j}),$$

where model ( $E(\mathbf{x}_i, t_{i,j}; \mathbf{P})$ ) and measurement ( $\hat{E}(\mathbf{x}_i, t_{i,j})$ ) errors are unknown and represented as random variables. Bayes' theorem is then applied to assimilate the concentration measurements and their uncertainties to produce a posterior distribution for the model parameters:

$$(5) \quad f_{\mathbf{P}}(\mathbf{p}|\{\hat{C}_{i,j}\}) = \frac{f_{\hat{C}}(\{\hat{C}_{i,j}\}|\mathbf{P} = \mathbf{p})f_{\mathbf{P}}(\mathbf{p})}{\int_{\Omega} f_{\hat{C}}(\{\hat{C}_{i,j}\}|\mathbf{P} = \mathbf{p})f_{\mathbf{P}}(\mathbf{p})d\mathbf{p}}$$

$$(6) \quad = \frac{f_{\hat{E}\mathbf{P}}(\{\hat{C}_{i,j} - C_{i,j}^{\mathbf{P}}\})f_{\mathbf{P}}(\mathbf{p})}{\int_{\Omega} f_{\hat{E}\mathbf{P}}(\{\hat{C}_{i,j} - C_{i,j}^{\mathbf{P}}\})f_{\mathbf{P}}(\mathbf{p})d\mathbf{p}}.$$

In (5), (6), and throughout, we employ the notational convenience of having  $\mathbf{P}$  denote a random variable and  $\mathbf{p}$  denote a (nonrandom) variable. In (5),  $f_{\hat{C}}(\{\hat{C}_{i,j}\}|\mathbf{P} = \mathbf{p})$  is the conditional, joint distribution of the measurements,  $\hat{C}_{i,j} \equiv \hat{C}(\mathbf{x}_i, t_{i,j})$  (the  $\{\cdot\}$  notation is used to indicate that the function is a function of all the  $\hat{C}_{i,j}$ ), and  $f_{\mathbf{P}}(\mathbf{p})$  is the joint prior distribution for the parameters. In (6),  $f_{\hat{E}\mathbf{P}}(\cdot)$  is the joint distribution of the model and measurement errors ( $\hat{E}_{i,j}^{\mathbf{P}} \equiv E(\mathbf{x}_i, t_{i,j}; \mathbf{P}) + \hat{E}(\mathbf{x}_i, t_{i,j})$ ). Note that in going from (5) to (6), we have reframed the conditional probabilities in terms of residuals and moved the dependence on  $\mathbf{p}$  from the conditional to the residual part. In general, this distribution may depend on  $\mathbf{p}$  in other ways, but in practice it is difficult to determine this dependence. Uncertainty in the conditional distribution will be dealt with using an information-gap uncertainty model.

Assuming that (1) there is no model inadequacy, (2) the conditional distribution is correct, and (3) there is sufficient data for the right-hand side of (5) and (6) to converge to  $f_{\mathbf{P}}(\mathbf{p})$ , it is possible to use the Bayesian approach to determine the probability that the contaminant concentration at  $\mathbf{x}_c$  at time  $t_c$  will be above  $C_c$ . From a numerical perspective this can be achieved by using a Markov chain Monte Carlo (MCMC) algorithm such as DREAM [18] to sample from the posterior distribution ( $f_{\mathbf{P}}(\mathbf{p}|\cdot)$ ) for  $\mathbf{P}$  and estimate the fraction of samples,  $\mathbf{P}_k$ , for which  $C_{\mathbf{P}_k}(\mathbf{x}_c, t_c) > C_c$ .

By introducing probability distributions for  $\mathbf{P}$  and  $\hat{E}_{i,j}^{\mathbf{P}}$ , the Bayesian approach attempts to resolve uncertainties in the parameters and the measurement errors. It even goes beyond the initial estimate for the uncertainty in the parameters (the prior distribution) by applying (5) to refine the distribution of  $\mathbf{P}$  based on the measured concentrations. However, the Bayesian approach ignores two important sources of uncertainty. First, it ignores model/conceptual uncertainty. For example, the model that is being used to represent reality may be an oversimplification that does not capture one or more critical physical processes. Second, it ignores the uncertainty in the conditional distribution of the measurements. For example, it may be

assumed that the  $E(\mathbf{x}_i, t_{i,j}; \mathbf{P}) - \hat{E}(\mathbf{x}_i, t_{i,j})$  obey a multivariate normal distribution with a particular mean and covariance, but in reality some other distribution may be more appropriate. This Bayesian approach does not attempt to resolve either of these uncertainties.

Another option for dealing with uncertainty is to use an information-gap approach [2, 6, 12]. Within the information-gap framework, there are innumerable possibilities. In [6], conceptual uncertainty in the contaminant source was considered, but broader parametric and model uncertainty were not considered. Uncertainty in the measurements was not explicitly considered as well. In [12], parametric and model/conceptual uncertainty were considered. Uncertainty in the measurements was not explicitly considered, and the accounting for parametric uncertainty was not as robust as in the Bayesian approach.

By combining the Bayesian approach with the information-gap approach, the individual shortcomings of these approaches can be circumvented to a large extent.

**2.1. Uncertainty in the distribution of errors.** The Bayesian approach accounts for some uncertainty in  $\hat{E}_{i,j}^{\mathbf{P}}$  but does not account for the uncertainty in what distribution to use to capture the uncertainty in  $\hat{E}_{i,j}^{\mathbf{P}}$ . For example, it is often assumed that errors obey a normal distribution. This assumption is best justified when the errors are a sum of many different error terms in the domain of attraction of the normal distribution (e.g., if it is a sum of a large number of independent, identically distributed terms with finite variance). Otherwise, the errors are not likely to be normally distributed. Even when the assumption of normality can be justified, there is still uncertainty in the mean, variance, and covariance. An information-gap model can be used to capture the uncertainty in the distribution.

We explore deviations in the distribution of the  $\hat{E}_{i,j}^{\mathbf{P}}$  from normality. Suppose that a nominal model for the distribution of  $\hat{E}_{i,j}^{\mathbf{P}}$  is multivariate normal with mean  $\mu_{i,j}$ , standard deviation  $\sigma_{i,j}$ , and covariance matrix  $\Sigma$ . One way to generalize the normal distribution to account for heavy tails while maintaining the central limit nature of the normal distribution is to use  $\alpha$ -stable Lévy distributions [13]. The  $\alpha$ -stable Lévy distributions are often denoted by  $S_\alpha(\lambda, \beta, \gamma)$ , having four parameters: the stability parameter ( $\alpha$ ), a scale parameter ( $\lambda$ ), a skewness parameter ( $\beta$ ), and a location parameter ( $\gamma$ ). When  $\alpha = 2$ , the distributions are normal distributions, and the skewness parameter becomes redundant. If  $X \sim N(\mu, \sigma^2)$ , then  $\mu + \frac{\sigma}{\sqrt{2}} F_{\alpha,\beta}^{-1}(F_2(\frac{X-\mu}{\sigma})) \sim S_\alpha(\sigma/\sqrt{2}, \beta, \mu)$  when  $\alpha \neq 1$  and  $F_{\alpha,\beta}(x)$  is the cumulative distribution function for the  $S_\alpha(1, \beta, 0)$  distribution and  $F_2(x)$  is the cumulative distribution function for the standard normal distribution. Note that  $S_\alpha(\lambda, \beta, \mu)$  has infinite standard deviation when  $\alpha < 2$ , and  $\lambda$  is never the standard deviation. The reason the factor of  $1/\sqrt{2}$  appears is that  $S_2(\sigma/\sqrt{2}, 0, \mu) \sim N(0, \sigma^2)$ .

This approach can be extended to a multivariate distribution by transforming each variable separately. The probability density function needed for (5) can then be computed via the chain rule. Assume that  $\hat{E}_{i,j}^{\mathbf{P}} \sim \mu_{i,j} + \frac{\sigma_{i,j}}{\sqrt{2}} F_{\alpha,\beta}^{-1}(F_2(\frac{X_{i,j} - \mu_{i,j}}{\sigma_{i,j}}))$ , where the  $X_{i,j}$  are normally distributed random variables with mean  $\mu_{i,j}$ , standard deviation  $\sigma_{i,j}$ , and covariance matrix  $\Sigma$ . Then, by a change of variables (see the appendix), the joint probability density function for the  $\hat{E}_{i,j}^{\mathbf{P}}$  is

$$(7) \quad f_{\hat{E}^{\mathbf{P}}}(\{\hat{E}_{i,j}^{\mathbf{P}}\}) = f_{\mu_{i,j}, \Sigma} \left( \left\{ \mu_{i,j} + \sigma_{i,j} F_2^{-1} \left( F_{\alpha,\beta} \left( \frac{\hat{E}_{i,j}^{\mathbf{P}} - \mu_{i,j}}{\sigma_{i,j}/\sqrt{2}} \right) \right) \right\} \right) \left| \det \frac{\partial \{X_{i,j}\}}{\partial \{\hat{E}_{i,j}^{\mathbf{P}}\}} \right|,$$

where  $f_{\mu_{i,j},\Sigma}(\mathbf{x})$  is the multivariate normal probability density function with mean  $\{\mu_{i,j}\}$  and covariance matrix  $\Sigma$ . Applying the inverse function theorem, the determinant is (see the appendix)

$$(8) \quad \left| \det \frac{\partial \{X_{i,j}\}}{\partial \{\hat{E}_{i,j}^{\mathbf{P}}\}} \right| = \left| \prod_{i \leq N_w} \prod_{j \leq N_{t,i}} \frac{\sqrt{2} f_{\alpha,\beta}(\sqrt{2}[\hat{E}_{i,j}^{\mathbf{P}} - \mu_{i,j}]/\sigma_{i,j})}{f_2(F_2^{-1}[F_{\alpha,\beta}(\sqrt{2}[\hat{E}_{i,j}^{\mathbf{P}} - \mu_{i,j}]/\sigma_{i,j})])} \right|,$$

where  $f_{\alpha,\beta}(x)$  is the probability density function for  $S_\alpha(1, \beta, 0)$ , and  $f_2$  is the probability density function for a standard normal distribution. Note that though  $\Sigma$  is not the covariance matrix of the  $\hat{E}_{i,j}^{\mathbf{P}}$ , it does define the interdependence between them. Denote a collection of random variables with the joint probability density function as given in (7) by  $MS_\alpha(\Sigma, \beta, \{\mu_{i,j}\})$ .

We can now define an information-gap uncertainty model that accounts for deviations from normality with heavy tails. Let

$$(9) \quad \mathcal{U}(\epsilon) = \left\{ MS_\alpha(C\Sigma, \beta, \{\mu_{i,j}\}), \alpha \in \left[ \max \left\{ \frac{1}{2}, \frac{1}{2} + \frac{3}{2 + \epsilon/5} \right\}, 2 \right], C \in [2^{-\epsilon}, 2^\epsilon] \right\}$$

be the information-gap uncertainty model capturing deviations from normality where  $\epsilon$  is the information-gap horizon of uncertainty. The nominal distribution ( $\epsilon = 0$ ) is  $N(\{\mu_{i,j}\}, \Sigma)$ . As the horizon of uncertainty,  $\epsilon$ , increases,  $\alpha$  is allowed to deviate further from 2 (producing potentially heavier tails) and  $\Sigma$  is rescaled by a bounded factor  $C$  with less restrictive bounds. The lower bound of 1/2 on  $\alpha$  in (9) is motivated by the numerics of (7), which can be problematic when  $\alpha$  is too close to 0. This is not a methodological limitation but just a computational convenience—if better numerical methods are available, the bound can be decreased.

A detailed demonstration of this uncertainty model will be exploited in section 3, but the basic idea will be presented here. Suppose it is necessary to decide whether or not to perform some remedial activity. With the Bayesian approach a decision to perform remediation would be made if, e.g., the probability of the concentration exceeding a maximum concentration limit (MCL) is greater than 5%. Suppose the Bayesian model is applied, and the result is that there is a 4% chance of exceeding the MCL. Given the uncertainties that are unaccounted for in the Bayesian approach, this number is uncertain, and therefore the appropriate decision is uncertain. By adding the information-gap model in (9), we can continue increasing  $\epsilon$  until there is an element in  $\mathcal{U}(\epsilon)$  that when used in (5) produces a probability of exceeding the MCL greater than 5%. If a large  $\epsilon$  is needed to make this happen, the decision is said to be robust. If a small  $\epsilon$  is sufficient, the decision is not robust and small deviations from the expected behavior can reverse the appropriate decision. In the latter case, it may be prudent to perform remediation, and a series of alternative remediation strategies can be evaluated. The remediation approach that produces the greatest robustness (i.e., the one that tolerates the greatest  $\epsilon$ ) would be preferred by information-gap decision theory.

**2.2. Model uncertainty.** Several issues arise when using parametric models, especially in a field like hydrology that is dominated by uncertainty: the dimensionality and extent of the parameter space are too great to fully explore the parameter space, the dimensionality and extent of the parameter space are too small to represent more complex possibilities, or

both of these issues exist at the same time. To overcome this, the uncertainty model that we employ to capture model uncertainty contains a set of models that are not parametric. The parametric models are included as a starting point in the uncertainty model. Define the uncertainty model

$$(10) \quad M(\epsilon, \mathbf{P}) = \left\{ C(\mathbf{x}, t) : \left| \frac{C(\mathbf{x}, t) - C_{\mathbf{P}}(\mathbf{x}, t)}{C_{\mathbf{P}}(\mathbf{x}, t)} \right| < \epsilon \right\}.$$

Let  $C^*(\mathbf{x}, t; \epsilon, \mathbf{P})$  denote the maximum concentration,

$$(11) \quad C^*(t; \epsilon, \mathbf{P}) = \max_{\mathbf{x} \in S_c, C \in M(\epsilon, \mathbf{P})} C(\mathbf{x}, t),$$

where  $S_c$  is a set of points of compliance (e.g., a supply well or a property boundary). As the horizon of uncertainty,  $\epsilon$ , increases, more models are included in  $M(\epsilon, \mathbf{P})$  and  $C^*(t; \epsilon, \mathbf{P})$  tends to increase. The probability density that we associate with  $M(\epsilon; \mathbf{P})$  is simply the density associated with the parameters  $\mathbf{P}$  in (5). This makes it possible to compute the probability that some  $C \in M(\epsilon, \mathbf{P})$  violates a compliance requirement, say that the concentration on the set  $S_c$  be below a threshold,  $C_c$ :

$$(12) \quad P(C^*(t; \epsilon, \mathbf{P}) > C_c) = \int_{\Omega} H\left(\frac{C^*(t; \epsilon, \mathbf{P})}{C_c} - 1\right) f_{\mathbf{P}}(\mathbf{P}|\{\hat{C}_{i,j}\})d\mathbf{P},$$

where  $H(x)$  is the Heaviside step function which is zero when  $x < 0$  and 1 when  $x \geq 0$ .

**2.3. Decision robustness and opportuneness.** When considering alternative remediation strategies, two basic situations can arise. Either the remediation is nominally successful (the probability of exceeding the MCL is less than 5%, assuming no model uncertainty and no uncertainty in the conditional distribution of errors) or nominally unsuccessful (the probability of exceeding the MCL is greater than 5%, assuming no model uncertainty and no uncertainty in the conditional distribution of errors).

If the remediation is nominally successful, it is natural to question the robustness of that success to uncertainty. The robustness is mathematically defined to be

$$(13) \quad R = \max \left\{ \epsilon : \left[ \max_{\{E_{i,j}\} \sim MS_{\alpha} \in \mathcal{U}(\epsilon)} P(C^*(t; \epsilon, \mathbf{P}) > C_c) \right] < 0.05 \right\}.$$

That is, the robustness is defined to be the maximum horizon of uncertainty at which the probability of failure is guaranteed to be less than 5%, accounting for the uncertainty in the application of Bayes' theorem (see (9)) and uncertainty in the model (through  $C^*$  from (10)). Conversely,  $R$  is how much uncertainty is required in order for it to be possible for the remediation goal (reducing the probability of failure below 5%) to fail.

If the remediation is nominally unsuccessful, it is natural to question how much opportunity there is for success given the uncertainty. The opportuneness is mathematically defined to be

$$(14) \quad O = \min \left\{ \epsilon : \left[ \min_{\{E_{i,j}\} \sim MS_{\alpha} \in \mathcal{U}(\epsilon)} P(C^*(t; \epsilon, \mathbf{P}) > C_c) \right] < 0.05 \right\}.$$

That is, the opportuneness is defined to be the minimum horizon of uncertainty at which the probability of failure can possibly be less than 5%, accounting for the uncertainty in the application of Bayes' theorem and uncertainty in the model. Conversely,  $O$  is how much uncertainty is required in order for it to be possible for the remediation goal to be achieved.

**3. Demonstration.** We now consider demonstrations of two synthetic contaminant remediation problems. The parametric model for the contaminant concentrations  $[M/L^3]$  is [11]

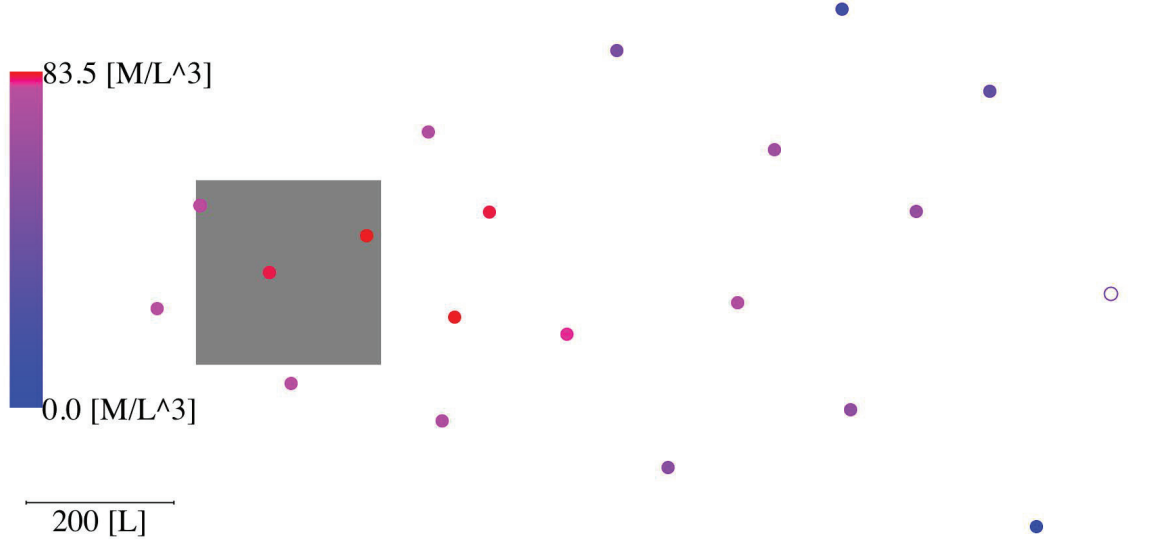
$$\begin{aligned}
 C(\mathbf{x}, t) = \frac{M}{8n\|B\|} \int_0^t \chi_{(0,1)}(t-\tau) \rho(\tau, t-\tau) & \left\{ \left[ \operatorname{erf} \left( \frac{x-x_1-v\tau}{\sqrt{4D_x\tau^{2H}}} \right) - \operatorname{erf} \left( \frac{x-x_2-v\tau}{\sqrt{4D_x\tau^{2H}}} \right) \right] \right. \\
 & \times \left[ \operatorname{erf} \left( \frac{y-y_1}{\sqrt{4D_y\tau}} \right) - \operatorname{erf} \left( \frac{y-y_2}{\sqrt{4D_y\tau}} \right) \right] \\
 & \times \left[ \operatorname{erf} \left( \frac{z-z_1}{\sqrt{4D_z\tau}} \right) - \operatorname{erf} \left( \frac{z-z_2}{\sqrt{4D_z\tau}} \right) \right. \\
 & \left. \left. + \operatorname{erf} \left( \frac{-z-z_1}{\sqrt{4D_z\tau}} \right) - \operatorname{erf} \left( \frac{-z-z_2}{\sqrt{4D_z\tau}} \right) \right] \right\} d\tau,
 \end{aligned}
 \tag{15}$$

where  $M$  is the contaminant mass flux  $[M/T]$ ,  $[x_1, x_2] \times [y_1, y_2] \times [z_1, z_2]$  is the region,  $B[L^3]$ , where the contaminant is released,  $n$  is the porosity  $[L^3/L^3]$ ,  $v$  is the mean velocity  $[L/T]$ ,  $D_x[L^2/T^{2H}]$ ,  $D_y$ , and  $D_z[L^2/T]$  are the dispersion coefficients in the  $x$ ,  $y$ , and  $z$  directions, respectively, and  $\|\cdot\|$  denotes volume. The model allows for the possibility of anomalous dispersion in the  $x$  direction via Brownian motion with Hurst exponent  $H$  [7]. The term  $\rho(\tau, t-\tau)$  represents the fraction of the contaminant mass released at time  $\tau$  that remains  $t-\tau$  time units after it was released.

**3.1. Scenario 1.** In this scenario, a contaminant is released from  $t=0$  to  $t=1[T]$ . The contaminant is monitored at 19 wells as  $t$  ranges from 0 to 10. Data for the contaminant concentrations at the monitoring wells are synthetic and were produced via a computer simulation. The observations for the contaminant concentrations at the monitoring wells are computed assuming that the contaminant source is box-shaped with a constant mass flux and the plume undergoes advection with a constant drift, classical dispersion in the  $y$  and  $z$  directions, fractional Brownian dispersion in the  $x$  direction, and first-order decay. Of course, in practice, the contaminant concentrations at the monitoring wells will come from measurements rather than simulations. At  $t=10$ , a decision must be made concerning the remediation of the contaminant. The desired outcome is that the contaminant concentration at a point of compliance is below the MCL,  $C_c$ , over the period from  $t=10$  to  $t=50$ . See Figure 1 for a depiction of the setup. The source has dimensions  $250 \times 250 \times 1 [L^3]$ .

Two remedial options are analyzed. One is the natural attenuation (NA) case, where it is deemed that naturally occurring biogeochemical reactions and dispersion are sufficient to reduce the contaminant concentrations below the MCL. The other is an approach to enhanced attenuation (EA), where a stimulant that converts the contaminant into an innocuous substance is injected into the contaminant plume (e.g., bioremediation). In the case of NA, first-





**Figure 1.** Network of wells and contaminant source for scenario 1. The 19 monitoring wells are shown with solid dots, the contaminant source location is represented with a square, and the point of compliance is shown by a hollow circle. The colors show the observed concentrations at  $t = 10 [T]$ .

order reactions are assumed so that

$$(16) \quad \rho(\tau, t - \tau) = e^{-\lambda_0(t-\tau)},$$

where  $\lambda_0$  is the naturally occurring reaction rate. For EA, the reaction rate is increased after  $t = 10[T]$  so that

$$(17) \quad \rho(\tau, t - \tau) = \begin{cases} e^{-\lambda_0(t-\tau)} & : t < 10, \\ e^{-\lambda_0(10-\tau)-\lambda_e(t-10)} & : t \geq 10, \end{cases}$$

where  $\lambda_e$  is the reaction rate after the remedial action has been taken.

The true values for the parameters in (15) are

$$(18) \quad M = 16 [M/T],$$

$$(19) \quad v = 16 [L/T],$$

$$(20) \quad H = 0.6 [-],$$

$$(21) \quad \lambda_0 = 0.01 [1/T],$$

$$(22) \quad \lambda_e = 0.02 [1/T],$$

$$(23) \quad (x_1, x_2) = (875, 1125) [L],$$

$$(24) \quad (y_1, y_2) = (1325, 1575) [L],$$

$$(25) \quad (z_1, z_2) = (0, 1) [L],$$

$$(26) \quad D_x = 1120 [L^2/T^{2H}],$$

$$(27) \quad (D_y, D_z) = (112, 22.4) [L^2/T].$$

The parameters are treated as nondimensional, but any consistent dimensionalization can be applied. For example, these parameters may be typical of a remedial scenario if mass is in kilograms, length is in meters, and time is in years. The MCL is

$$(28) \quad C_c = 10 [M/L^3].$$

Parametric uncertainty is considered in the naturally occurring reaction rate ( $\lambda_0$ ) and the mechanism of longitudinal aquifer dispersion ( $H$ ). The prior distribution for  $\lambda_0$  is uniform over the interval  $[0, 1]$ . The prior distribution for  $H$  is uniform over the interval  $[1/2, 1]$ , which allows the possibility for the longitudinal dispersion to be classical ( $H = 0.5$ ) or highly superdispersive ( $H$  near 1). The parameters for the nominal conditional distribution ( $N(\{\mu_{i,j}\}, \Sigma)$ ) are  $\mu_{i,j} = 0$  and  $\Sigma = I$  (where  $I$  is the identity matrix).

In summary, there are 10 contaminant concentrations observed at each of 20 monitoring wells representing 200 data records. There are two uncertain model parameters with distributions informed via Bayes' theorem by the observed concentration data. The decision analysis proceeds by computing the robustness,  $R$ , from (13). Conceptually, this can be understood to consist of three nested loops. The outer loop iterates over increasing values of the horizon of uncertainty,  $\epsilon$ . The middle loop iterates over possible conditional distributions in  $\mathcal{U}(\epsilon)$  from (9). The inner loop performs an MCMC iteration to sample from the posterior distribution for the parameters. The samples are used to compute the probability of failure given the model uncertainty,  $M(\epsilon, \mathbf{P})$  from (10).

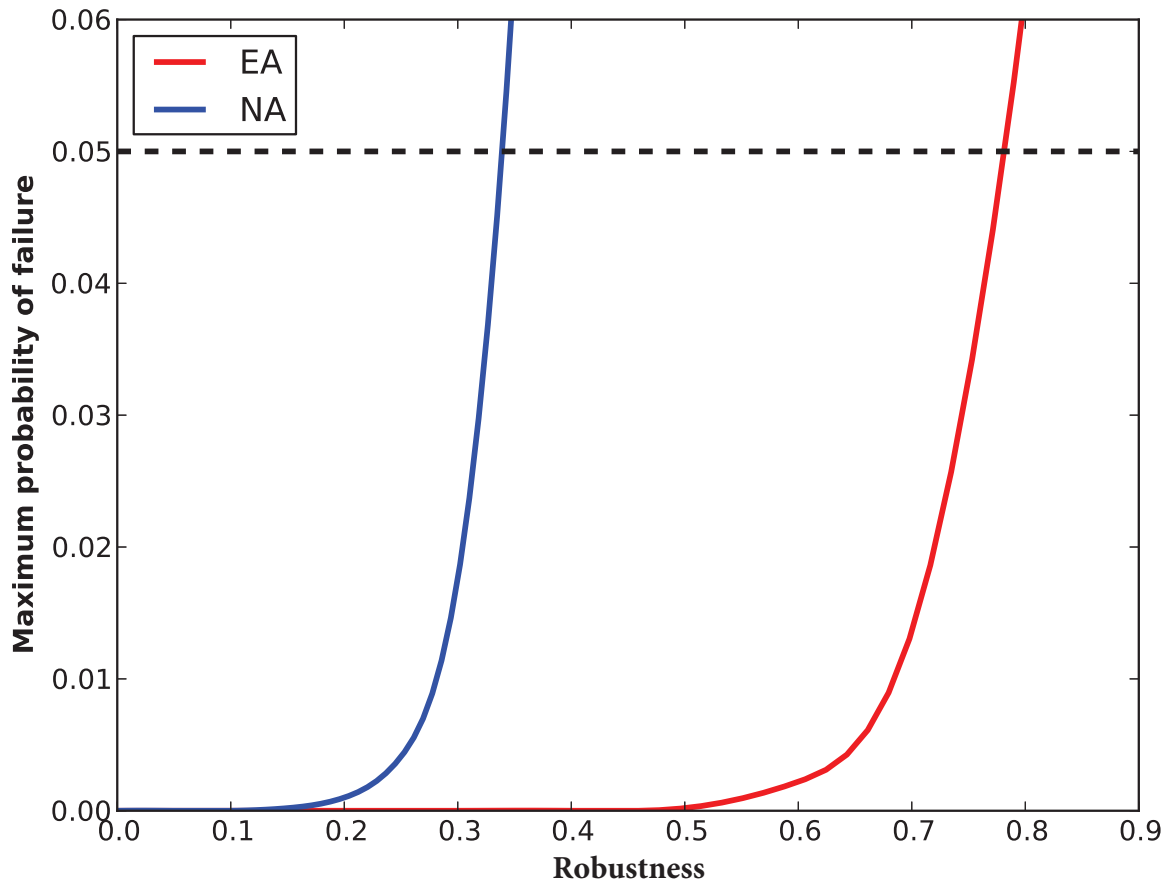
The decision-analysis results suggest that for both the NA and the EA scenarios, the nominal probability of failure is approximately zero. That is, when  $\epsilon = 0$ , the inner maximum in (13) is approximately zero. Figure 2 depicts the robustness (horizontal) versus acceptable probability of failure (inner maximum in (13)). The robustness,  $R$ , is found by locating the value of  $\epsilon$  where the curves intersect the dashed line in Figure 2. The values of  $R$  for the NA and EA scenarios are 0.34 and 0.78, respectively. This indicates that substantially more uncertainty is required in order for the failure of EA to be possible. The robustness value of 0.34 for NA means that the concentrations may exceed the MCL with only a 34% model error and within a relatively small window around the nominal conditional distribution. Relative to the severe uncertainties typically present in subsurface remediation problems, this is a modest amount of uncertainty. Therefore, and despite the fact that the nominal probability of failure for NA is nearly zero, it would be prudent in this scenario to perform the EA remediation strategy. The maximum probability of EA failure increases rapidly for  $\epsilon \approx R$ , providing further support for this perspective.

**3.2. Scenario 2.** The second scenario is similar to the first with the following modifications. The mean velocity and the contaminant mass flux rate have been modified:

$$(29) \quad M = 256 [M/T],$$

$$(30) \quad v = 110 [L/T].$$

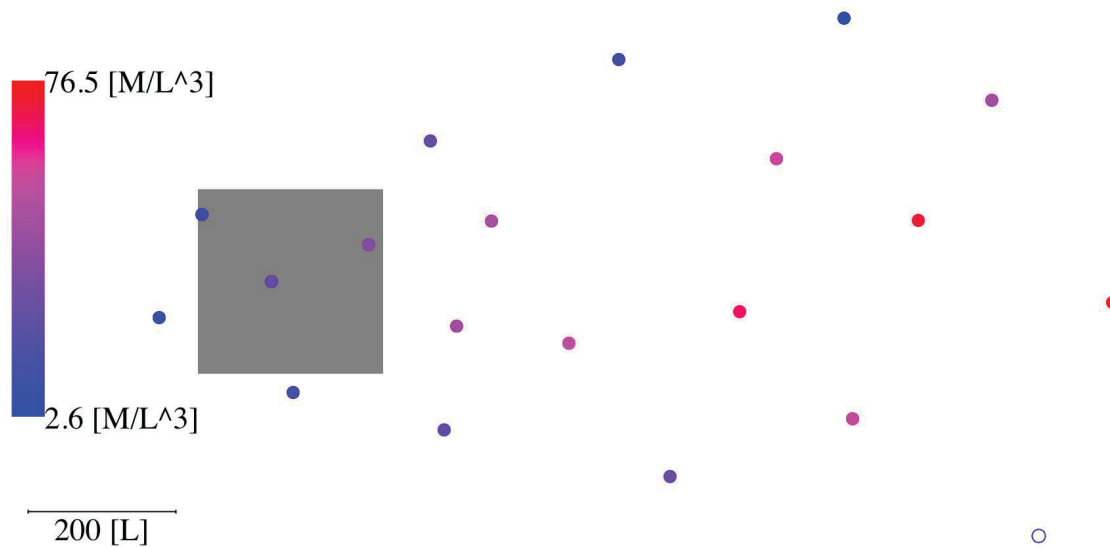
The compliance point has been relocated, and it is not aligned with the transport direction of the contaminant plume center of mass (compare Figure 3 to Figure 1). Figure 4 plots the robustness (horizontally) as a function of the maximum chance of failure (vertically). In this



**Figure 2.** The robustness (horizontally) as a function of the maximum chance of failure (vertically) for scenario 1. With both remediation approaches, the nominal ( $\epsilon = 0$ ) chance of failure is approximately zero. However, the maximum chance of failure remains low over a substantially larger uncertainty range for EA compared to NA.

scenario, both remediation approaches have a small chance of failure over a relatively large range. The robustness for the EA approach is approximately 1.35, compared to 1.34 for the NA approach. In this scenario, the NA approach is likely to succeed even after allowing for substantial modeling error (134% model error) as well as a relatively broad neighborhood around the nominal conditional distribution used in Bayes' theorem. Therefore, the NA approach may be sufficient in this case. The EA approach provides only a very small amount of additional robustness. Therefore, it is not a strong alternative to the NA approach. If the robustness provided by NA is insufficient, the robustness provided by EA is very likely to be insufficient as well. In this case, it would be prudent to find an alternative remediation approach.

In this scenario, the decision analyses suggest that the EA does not substantially increase the robustness. By the time the EA has been implemented, the peak concentrations have already been observed at the compliance point. The aquifer dispersion has a much stronger



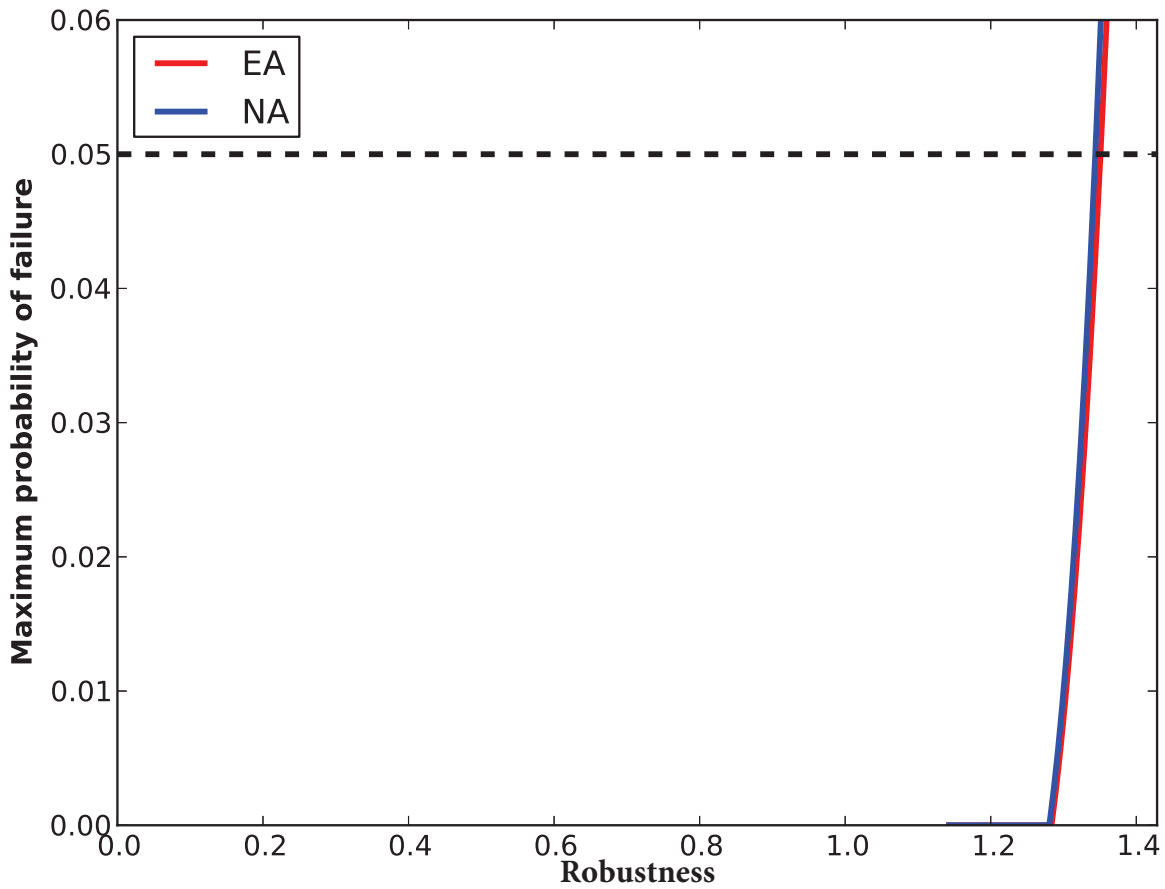
**Figure 3.** Network of wells and contaminant source for scenario 2. The 19 monitoring wells are shown with filled-in circles, the contaminant source location is represented with a square, and the point of compliance is shown by a hollow circle. The colors show the observed concentrations at  $t = 10$  [T].

impact on reducing the contaminant concentrations at the point of compliance than increasing the reaction rate. In this scenario, it would not be prudent to perform the EA. If the robustness provided by NA is deemed insufficient, an alternative remediation approach should be pursued.

**4. Conclusion.** Unknowns and uncertainty play a significant role in selecting a remedy for contaminated groundwater. Measurement errors, parametric uncertainties, and model inadequacies all contribute to these unknowns and uncertainties. We have described a decision support framework that takes these unknowns and uncertainties into consideration. The framework consists of three layers. The inner layer uses a nonprobabilistic, information-gap approach to overcome model inadequacy. The middle layer uses Bayes' theorem to account for uncertainty in the parameters and the measurements based on prior information about the probability density distributions and field measurements. The outer layer considers uncertainty in the application of Bayes' theorem.

The framework was demonstrated in two scenarios. For demonstration purposes, a model was used to generate concentration "measurements" at 20 observation wells (including the compliance point) and at 10 times each. To make the scenarios realistic, the 200 concentration measurements and the prior parameter distributions are used to inform the decision analysis, but no additional information about the model is supplied. In one case, natural attenuation (NA) was substantially less robust than the preferred enhanced attenuation (EA) approach. In the other, there was little benefit in performing the EA, and the NA should be the preferred remedial action.

The framework represents a general, comprehensive, and novel approach for dealing with a diverse range of uncertainties and unknowns associated with model-based decision analyses.



**Figure 4.** The robustness (horizontally) as a function of the maximum chance of failure (vertically) for scenario 2. Note that in this scenario, the EA approach provides little additional robustness.

Applications of this approach are not limited to groundwater remediation problems. It can be applied to engineering fields that combine data and models to make decisions, e.g. climate change, energy production, waste storage, carbon sequestration, etc.

**Appendix. Change of variables calculation.** If  $\mathbf{X} = (X_1, X_2, \dots, X_n)$  is an  $n$ -dimensional random variable and  $G(\mathbf{X}) = \mathbf{Y} = (Y_1, Y_2, \dots, Y_n)$  is another  $n$ -dimensional random variable, then

$$(31) \quad f_{\mathbf{Y}}(\mathbf{y}) = f_{\mathbf{X}}(G^{-1}(\mathbf{y})) |\det J[G^{-1}](\mathbf{y})|,$$

where  $f_{\mathbf{Y}}(\mathbf{y})$  is the probability density function for  $\mathbf{Y}$ ,  $f_{\mathbf{X}}(\mathbf{x})$  is the probability density function for  $\mathbf{X}$ , and  $J$  denotes the Jacobian operator. In the case of (7), the transformation can be decomposed as  $Y_i = G_i(X_i)$ , where

$$(32) \quad G_i(X_i) = a_i + \frac{b_i}{\sqrt{2}} F_1^{-1} \left( F_2 \left( \frac{X_i - a_i}{b_i} \right) \right).$$

This implies that  $G^{-1}(\mathbf{y})$  can also be decomposed componentwise:

$$(33) \quad G_i^{-1}(Y_i) = a_i + b_i F_2^{-1} \left( F_1 \left( \frac{Y_i - a_i}{b_i/\sqrt{2}} \right) \right).$$

Inserting this into (31) establishes (7). It remains to establish (8), that is, to compute the determinant. Observe that  $J(H^{-1})$  is diagonal, because  $G_i$  depends only on  $Y_i$ , and not  $Y_j$  for  $j \neq i$ . Therefore, the absolute value of the determinant is the absolute value of the product of the  $(G_i^{-1})'(Y_i)$ . Differentiating (33) is a calculus exercise that utilizes the chain rule and the inverse function theorem:

$$(34) \quad (G_i^{-1})'(Y_i) = b_i (F_2^{-1})' \left( F_1 \left( \frac{Y_i - a_i}{b_i/\sqrt{2}} \right) \right) F_1' \left( \frac{Y_i - a_i}{b_i/\sqrt{2}} \right) \frac{1}{b_i/\sqrt{2}}$$

$$(35) \quad = \frac{\sqrt{2} F_1' \left( \frac{Y_i - a_i}{b_i/\sqrt{2}} \right)}{F_2' \left( F_2^{-1} \left( F_1 \left( \frac{Y_i - a_i}{b_i/\sqrt{2}} \right) \right) \right)}.$$

Combined with the previous results on the diagonality of the Jacobian, this establishes (8).

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