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Multiple Predictor Smoothing Methods for Sensitivity Analysis: Example Results

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Abstract

The use of multiple predictor smoothing methods in sampling-based sensitivity analyses of complex models is investigated. Specifically, sensitivity analysis procedures based on smoothing methods employing the stepwise application of the following nonparametric regression techniques are described in the first part of this presentation: (i) locally weighted regression (LOESS), (ii) additive models, (iii) projection pursuit regression, and (iv) recursive partitioning regression. In this, the second and concluding part of the presentation, the indicated procedures are illustrated with both simple test problems and results from a performance assessment for a radioactive waste disposal facility (i.e., the Waste Isolation Pilot Plant). As shown by the example illustrations, the use of smoothing procedures based on nonparametric regression techniques can yield more informative sensitivity analysis results than can be obtained with more traditional sensitivity analysis procedures based on linear regression, rank regression or quadratic regression when nonlinear relationships between model inputs and model predictions are present.

Key Words: Additive models, Epistemic uncertainty, Locally weighted regression, Nonparametric regression, Projection pursuit regression, Recursive partitioning regression, Scatterplot smoothing, Sensitivity analysis, Stepwise selection, Uncertainty analysis.

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1. Introduction

The first part of this presentation[1] reviews parametric and nonparametric regression procedures for use in sampling-based sensitivity analyses. Specifically, the following parametric regression procedures are introduced and briefly described in Sect. 2 of Ref. 1: (i) linear regression (LIN_REG), (ii) rank regression (RANK_REG), and (iii) quadratic regression (QUAD_REG). Further, the following nonparametric regression procedures are introduced and briefly described in Sect. 3.3 of Ref. 1: (i) locally weighted regression (LOESS), (ii) additive models (GAMs), (iii) projection pursuit regression (PP_REG), and (iv) recursive partitioning regression (RP_REG). In addition, algorithms for the stepwise implementation of these procedures in the R language as part of a sensitivity analysis are described in Sect. 4 of Ref. 1.

The efficacy of the various methods described in Ref. 1 as procedures for sensitivity analysis is now investigated with both analytic test model data and real data. The analytic test models were assembled as part of a review volume on sensitivity analysis.[2, 3] The real data comes from a performance assessment for the Waste Isolation Pilot Plant (WIPP).[4, 5] The methods are compared on the basis of fidelity to the data, overfitting of the data, and reproducibility.

The presentation is organized as follows. First, certain quantities used in assessing the efficacy of the various sensitivity analysis procedures are introduced (Sect. 2). Then, the results obtained with the analytic test models are presented (Sect. 3). Next, the results obtained with the data from the WIPP performance assessment are presented (Sect. 4). The presentation then ends with a summary of observations and insights (Sect. 5).

2. Assessment of Analysis Efficacy

The R^2 statistic (see Eq. (2.5), Ref. 1) provides one measure of the fidelity of a regression model to the data from which it was constructed. In particular, the closer R^2 is to one, the better the model reproduces the data. However, the R^2 statistic can be misleading in that its value can be unrealistically inflated by overfitting the data. The adjusted R^2 statistic R_A^2 provides a measure of fidelity that attempts to correct the effects of overfitting the data (pp. 91 – 92, Ref. 6). Specifically, R_A^2 is defined by

$$R_A^2 = 1 - \frac{(nS-1)\sum_{i=1}^{nS}(\hat{y}_i - y_i)^2}{(nS-p)\sum_{i=1}^{nS}(y_i - \bar{y})^2} = 1 - \left(1-R^2\right)\left(\frac{nS-1}{nS-p}\right), \tag{2.1}$$

where p is the number of degrees of freedom associated with the fitted model. However, the values for R^2 and R_A^2 are similar when p is small relative to nS.

The PRESS statistic *PRS* (see Eq. (3.19), Ref. 1) provides a way to test for an overfitting of the data. In particular, a decrease in *PRS* with the addition of a variable to a model indicates an improvement in the predictive capability of the model (i.e., the fidelity of the model to the data has increased). In contrast, an increase in *PRS* indicates that an overfitting of the data has taken place. This property results because the PRESS statistic is very sensitive to the effects of a limited number of highly influential observations (typically observations with extreme values for one or a few independent variables). Monitoring PRESS values as variables are added to a model provides a way to check for overfitting of the data, with such overfitting indicated when the addition of a variable results in an increase in the PRESS value over the PRESS value obtained before the addition of that variable. Such a jump in the PRESS statistic indicates the model is starting to “chase” results associated with individual observations rather than following actual patterns in the data.

The PRESS statistic can also be used to compare the fidelity of models constructed from the same data set but with different procedures. In particular, a model with a lower PRESS value is preferable to a model with a higher PRESS value. However, there are two drawbacks in using PRESS to compare models obtained with different procedures. First, PRESS values can be very sensitive to the effects of a limited number of extreme observations. Second, there is no “absolute” standard against which a PRESS value can be compared to indicate whether or not a model is providing a good match to the data. In contrast, R^2 values approach one as the fidelity of the model to the data increases; unfortunately, there is no such limiting value for the PRESS statistic.

The adjusted PRESS value PRS_A (see Eqs. (3.22) – (3.25), Ref. 1) reduces the effects of highly influential observations by using an average leverage value in its definition. The adjusted PRESS value PRS_A is similar in concept to the adjusted R^2 value R_A^2 in that it penalizes a model for the use of an excessive number of degrees of freedom in its construction. However, as with the original statistic *PRS*, there is no limiting value for PRS_A that provides a standard by which the fidelity of a model to the underlying data can be judged. Although PRS_A can be more useful than the original PRESS statistic in comparing models constructed with different procedures, it is less effective in checking for overfitting because of the reduction in the effects of extreme observations.

The top-down coefficient of concordance (TDCC) provides a way to assess the reproducibility of sensitivity analysis results obtained with individual analysis procedures.[7, 8] In particular, the TDCC provides a measure of the agreement between results obtained with independently generated samples in a manner that emphasizes agreement in the identification of the most important variables and places less emphasis on agreement in the identification of the less important variables. For notational purposes in the definition of the TDCC, suppose (i) nR independently generated samples of the same size involving a vector $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$ of independent variables are under consideration, (ii) a sensitivity analysis to rank variable importance is carried out for each sample, and (iii) r_{jk} denotes the rank assigned to variable j in the indicated sensitivity analysis for sample k, where the most important variable is assigned a rank of 1, the next most important variable is assigned a rank of 2, and so on, with variables of the same importance assigned their average rank (the preceding is the reverse of the ranking procedure described in Sect. 2.2 of Ref. 1 for rank regression). The TDCC is then defined by

$$C_T = \left\{ \sum_{j=1}^{nX} \left[\sum_{k=1}^{nR} ss\left(r_{jk}\right) \right]^2 - \left(nR\right)^2 nX \right\} \Bigg/ \left\{ \left(nR\right)^2 \left(nX - \sum_{j=1}^{nX} 1/j \right) \right\}, \tag{2.2}$$

where $ss(r_{jk})$ is the Savage score given by

$$ss\left(r_{jk}\right) = \sum_{i=r_{jk}}^{nX} 1/i$$

for variable j in a sample k and average Savage scores are assigned in the event of ties. Use of the Savage scores $ss(r_{jk})$ rather than the ranks r_{jk} in the definition of the TDCC in Eq. (2.2) results in the previously indicated emphasis on agreement on the most important variables and deemphasis on disagreement on the less important variables.

In the examples that follow, variable importance is defined by the order in which variables enter the model under construction, with the first variable entering the model ranked 1, the second variable entering the model ranked 2, and so on. The variables that are not selected for entry into the model are all assigned the same average rank. The preceding ranking is used in the calculation of the TDCC. Values for the TDCC close to one indicate a high level of reproducibility for the sensitivity analysis method under consideration, with a decrease in reproducibility indicated as the value for the TDCC decreases away from one.

The primary emphasis of this presentation is on regression-based procedures for sensitivity analysis. For comparison, a nonregression-based procedure for sensitivity analysis is also included. This procedure is referred to as the SRD/RCC test and is the result of combining a test for nonrandomness in the relationship between an independent and a dependent variable called the squared rank differences (SRD) test with the Spearman rank correlation coefficient (RCC).[9] This test is effective at identifying linear and very general nonlinear patterns in analysis results. However, unlike the regression procedures under consideration, the SRD/RCC test does not involve the development of a model that approximates the relationship between independent and dependent variables.

A brief description of the SRD/RCC test follows. The test is used to assess the relationships between individual elements x_j of $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$ and a predicted variable y of interest for a random or LHS and a functional relationship of the form indicated in Eq. (1.8) of Ref. 1. The SRD component of the test is based on the statistic

$$Q_j = \sum_{i=1}^{nS-1} \left(r_{j,i+1} - r_{ji}\right)^2, \tag{2.3}$$

where r_{ji}, $i = 1, 2, \ldots, nS$, is the rank of y obtained with the sample element in which x_j has rank i and the indicated ranks are defined as described in Sect. 2.2 of Ref. 1. Under the null hypothesis of no relationship between x_j and y, the quantity

$$S_j = \left\{Q_j - \left[nS\left(nS^2 - 1\right)/6\right]\right\} \Big/ \left\{\sqrt{nS^5}/6\right\} \tag{2.4}$$

approximately follows a standard normal distribution for $nS > 40$. Thus, a p-value p_{rj} indicative of the strength of the nonlinear relationship between x_j and y can be obtained from Q_j. Specifically, p_{rj} is the probability that a value $\tilde{Q}_j > Q_j$ would occur due to chance if there was no relationship between x_j and y. The RCC component of the test is based on the rank (i.e., Spearman) correlation coefficient

$$R_j = \frac{\sum_{i=1}^{nS}\left[R\left(x_{ij}\right) - \left(nS+1\right)/2\right]\left[R\left(y_i\right) - \left(nS+1\right)/2\right]}{\left\{\sum_{i=1}^{nS}\left[R\left(x_{ij}\right) - \left(nS+1\right)/2\right]^2\right\}^{1/2}\left\{\sum_{i=1}^{nS}\left[R\left(y_i\right) - \left(nS+1\right)/2\right]^2\right\}^{1/2}}, \tag{2.5}$$

where $R(x_{ij})$ and $R(y_i)$ are the ranks associated x_j and y for sample element i. Under the null hypothesis of no rank correlation between x_j and y, the quantity R_j has a known distribution (Table A10, Ref. 10). Thus, a p-value p_{cj} indicative of the strength of the monotonic relationship between x_j and y can be obtained from R_j. The SRD/RCC test is obtained from combining the p-values p_{rj} and p_{cj} to obtain the statistic

$$\chi_4^2 = -2\left[\ln\left(p_{rf}\right) + \ln\left(p_{cj}\right)\right], \tag{2.6}$$

which has a chi-squared distribution with four degrees of freedom. The p-value associated with χ_4^2 constitutes the SRD/RCC test for the strength of the relationship between x_j and y. A detailed description of the SRD/RCC test and the determination of the associated p-value is available elsewhere.[9]

3. Example Results: Analytic Test Models

Results obtained with the following four analytic test models are now presented:

$$y_1 = f_1\left(x_1, x_2\right) = 5x_1 + \left(5x_2\right)^4, \tag{3.1}$$

$$y_2 = f_2\left(x_1, x_2\right) = \left(x_2 + 0.5\right)^4 \Big/ \left(x_1 + 0.5\right)^2, \tag{3.2}$$

$$y_3 = f_3\left(x_1, x_2, \ldots, x_8\right) = \prod_{j=1}^{8}\left\{\frac{\left|4x_j - 2\right| + a_j}{1 + a_j}\right\} \tag{3.3}$$

with $[a_1, a_2, \ldots, a_8] = [0, 1, 4.5, 9, 99, 99, 99, 99]$, and

$$\begin{aligned} y_4 &= f_4(x_1, x_2, x_3) \\ &= \sin(2\pi x_1 - \pi) + 7\sin^2(2\pi x_2 - \pi) + 0.1(2\pi x_3 - \pi)^4 \sin(2\pi x_1 - \pi). \end{aligned} \tag{3.4}$$

The individual models have from 2 to 8 input variables that are assumed to be uniformly and independently distributed on [0, 1]. The functions f_1, f_2, f_3 and f_4 and the associated distributional assumptions for the x_j's correspond to Model 4c, 6b, 7 and 9, respectively, in Ref. 3. The functions f_1, f_3 and f_4 are also considered in Sects. 4 and 5 of Ref. 11.

The example analyses use three replicated random samples of size 100 each from 10 variables (i.e., the x_j) with uniform distributions on [0, 1]. This results in the analysis for each model including from 2 to 8 completely spurious variables. The presence of such variables provides an indication of whether or not the individual regression procedures have a tendency to include spurious variables in model construction. As for the WIPP example (Sect. 4), the replicated sampling results in the three samples of the form indicated in Eq. (1.5) of Ref. 1 and three mappings of the form indicated in Eq. (1.6) of Ref. 1. As in Sect. 4, the individual replicates are referred to as replicates R1, R2 and R3, respectively.

In concept, the example results can be thought of as the outcome of evaluating a model of the form

$$y = f(\mathbf{x}) = [f_1(\mathbf{x}), f_2(\mathbf{x}), f_3(\mathbf{x}), f_4(\mathbf{x})] \tag{3.5}$$

with $\mathbf{x} = [x_1, x_2, \ldots, x_{10}]$. Such multiple outcomes are usually the case in analyses of real systems (e.g., see the analyses in Refs. 12-14 from which the examples in Sect. 4 are derived). Further, it is also typical of such analyses that individual results are not affected by all of the uncertain variables under consideration.

The analytic models introduced in this section (Sect. 3) have an advantage over the real model considered in the following section (Sect. 4) in that it is possible to unambiguously determine the contributions of individual analysis inputs to the uncertainty in analysis results. This is not possible with a computationally demanding model of the type considered in Sect. 4. In particular, such determinations make comparisons between truth and sensitivity results obtained with the procedures under consideration possible. The method used to determine the actual effects of individual variables is described in the next paragraph.

The R^2 value is the primary quantity used in this presentation to assess the contribution of the uncertainty associated with a group of variables to the uncertainty in an analysis result. In particular, if $\tilde{\mathbf{x}} = [\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_p]$ is a vector of variables taken from the variables $x_1, x_2, \ldots, x_{nX}$ under consideration in a particular analysis (i.e., $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$ is the vector of uncertain inputs under consideration), $\hat{f}(\tilde{\mathbf{x}}) = \hat{f}(\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_p)$ is an approximation to the real model $f(\mathbf{x}) = f(x_1, x_2, \ldots, x_{nX})$ estimated with a particular procedure from a mapping $[\mathbf{x}_i, y_i]$, $i = 1, 2, \ldots nS$, from analysis inputs to analysis results, and $\tilde{\mathbf{x}}_i = [\tilde{x}_{i1}, \tilde{x}_{i2}, \ldots, \tilde{x}_{ip}]$ for $i = 1, 2, \ldots, nS$, then

$$R^2 = 1 - \sum_{i=1}^{nS}\left[y_i - \hat{f}\left(\tilde{\mathbf{x}}_i\right)\right]^2 \Big/ \sum_{i=1}^{nS}\left[y_i - \bar{y}\right]^2 \tag{3.6}$$

provides an estimate of the fraction of the uncertainty in y that derives from the uncertainty associated with the variables in $\tilde{\mathbf{x}}$.

The contribution of $\tilde{\mathbf{x}}$ to the uncertainty in y that is estimated by R^2 is formally defined by the correlation ratio

$$\begin{aligned}\eta^2 &= 1 - E\left(\left[y - E\left(y|\tilde{\mathbf{x}}\right)\right]^2\right) \Big/ E\left(\left[y - E\left(y\right)\right]^2\right)\\ &= 1 - E\left[Var\left(y|\tilde{\mathbf{x}}\right)\right] / Var\left(y\right)\\ &= Var\left[E\left(y|\tilde{\mathbf{x}}\right)\right] / Var\left(y\right),\end{aligned} \tag{3.7}$$

where (i)

$$E(y) = \int_X f(\mathbf{x})\, d_X(\mathbf{x})\, \mathrm{d}X$$

$$E\left(y|\tilde{\mathbf{x}}\right) = \int_{\tilde{X}^c} f\left(\tilde{\mathbf{x}}^c, \tilde{\mathbf{x}}\right) d_{\tilde{X}^c}\left(\tilde{\mathbf{x}}^c\right) \mathrm{d}\tilde{X}^c$$

$$E\left(\left[y - E(y)\right]^2\right) = \int_X \left[f(\mathbf{x}) - E(y)\right]^2 d_X(\mathbf{x})\, \mathrm{d}X = Var(y)$$

$$E\left(\left[y - E\left(y|\tilde{\mathbf{x}}\right)\right]^2\right) = \int_X \left[f(\mathbf{x}) - E\left(y|\tilde{\mathbf{x}}\right)\right]^2 d_X(\mathbf{x})\, \mathrm{d}X = E\left[Var\left(y|\tilde{x}\right)\right]$$

$$Var\left[E\left(y|\tilde{\mathbf{x}}\right)\right] = \int_{\tilde{X}} \left[E\left(y|\tilde{\mathbf{x}}\right) - E(y)\right]^2 d_{\tilde{X}}(\tilde{\mathbf{x}})\, \mathrm{d}\tilde{X},$$

(ii) $(\mathcal{X}, \mathbb{X}, p_X)$, $(\tilde{\mathcal{X}}, \tilde{\mathbb{X}}, p_{\tilde{X}})$ and $(\tilde{\mathcal{X}}^c, \tilde{\mathbb{X}}^c, p_{\tilde{X}^c})$ are the probability spaces associated with $\mathbf{x}$, $\tilde{\mathbf{x}}$, and $\tilde{\mathbf{x}}^c$, where $\tilde{\mathbf{x}}^c$ contains the elements of $\mathbf{x}$ not contained in $\tilde{\mathbf{x}}$, and (iii) $d_X(\mathbf{x})$, $d_{\tilde{X}}(\tilde{\mathbf{x}})$ and $d_{\tilde{X}^c}(\tilde{\mathbf{x}}^c)$ are the corresponding density functions for $\mathbf{x}$, $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{x}}^c$ (Sect. 8.2, Ref. 15). The quantity η^2 is based on the analysis of variance (ANOVA) decomposition

$$Var(y) = Var\left[E\left(y|\tilde{\mathbf{x}}\right)\right] + E\left[Var\left(y|\tilde{\mathbf{x}}\right)\right] \tag{3.8}$$

and corresponds to the fraction of the variance of y that derives from the uncertainty associated with the variables that constitute the elements of $\tilde{\mathbf{x}}$.[15-19] For the simple functions considered in this section, η^2 can be calculated and used in comparisons with its corresponding estimate R^2 defined in Eq. (3.6). In some cases, the estimate R^2 can be shown to converge in probability to η^2 as $n \to \infty$.[20, 21]

In the following, η^2 is calculated in a stepwise manner for use in determining variable importance. The most important variable, designated $\tilde{x}_1$, is the element of $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$ that gives the largest value for η^2. That is, $\tilde{\mathbf{x}} = [x_1]$, $\tilde{\mathbf{x}} = [x_2]$, …, $\tilde{\mathbf{x}} = [x_{nX}]$ are considered in the definition of η^2 in Eq. (3.7), and the x_j that gives the highest value for η^2 is deemed to be the most important variable and taken to be $\tilde{x}_1$. The second most important variable, designated $\tilde{x}_2$, is the element of $\mathbf{x} = [x_1, x_2, \ldots, x_{nX}]$ that gives the largest value for η^2 when all possible values for $\tilde{\mathbf{x}} = [\tilde{x}_1, x_j]$, $\tilde{x}_1 \neq x_j$, are considered. The third most important variable, designated $\tilde{x}_3$, is determined in like manner from consideration of vectors of the form $\tilde{\mathbf{x}} = [\tilde{x}_1, \tilde{x}_2, x_j]$, $\tilde{x}_1 \neq x_j$ and $\tilde{x}_2 \neq x_j$, and so on through all nX elements of $\mathbf{x}$.

The individual analytical test models are now considered. For each test problem, R^2, R_A^2, PRS, PRS_A, and the TDCC C_T are calculated for the following methods: LIN_REG, RANK_REG, QUAD_REG, LOESS, PP_REG, RP_REG and GAM. The TDCC is calculated from the three replicated samples of size 100, and the rest of the results are calculated from the pooled sample of size 300. For comparison, the true η^2 values are also presented. The TDCC score comparing the variable rankings obtained with each method with the rankings based on the true model are also given.

3.1 Monotonic Relationships: $y_1 = f_1(x_1, x_2)$

The uncertainty in y_1 is mainly driven by x_2 as can be seen in Fig. 1. The results of the various regression methods applied to y_1 are given in Table 1. As indicated by the analysis for the true model in Table 1 (i.e., in the value of η^2 defined in Eq. (3.7)), 99.99% of the uncertainty in y_1 is due to x_2. All the analysis methods agree with the true model in the identification of x_2 as the most important variable. The analysis with LIN_REG has some trouble with a failure to include x_1 in the model and an R^2-value of only 0.76. In contrast, RANK_REG does better as the underlying relationships are monotonic and results in a model containing both x_1 and x_2 and a final R^2 value of 0.98. The analyses with QUAD_REG and LOESS successfully estimate the contribution of x_2 with R^2 values of 0.98 and 1.00, respectively, but fail to identify the effect of x_1. The analyses with PP_REG, GAM and RP_REG all do well in that they include x_1 and x_2 and also give R^2 values for x_1 and x_2 that are equal to the values obtained for the true model. However, PP_REG includes the spurious variables x_5 and x_7. The non-regression based method SRD/RCC also identifies both x_1 and x_2 as important variables. The analysis of y_1 is challenging with respect to the identification of x_1 due to the very small effect associated with this variable.

3.2 Monotonic Relationships: $y_2 = f_2(x_1, x_2)$

All of the regression methods identify the two important variables (i.e., x_1 and x_2) for y_2 (Fig. 2). As shown in Table 2, the regression methods all indicate that x_2 is the most important variable followed by x_1, which results in a high TDCC with the true model for all the methods. The analysis with LIN_REG underestimates the contribution of x_1. The analysis with RANK_REG overestimates the contribution of x_2; this is likely because rank transformed data instead of actual the y values are being used to compute R^2. The analysis with GAM underestimates x_1's contribution because of its inability to model interactions. The analyses with QUAD_REG, PP_REG, LOESS, and RP_REG give good estimates of the R^2 contribution of x_2 and x_1. However, the analyses with GAM and RP_REG each include one spurious variable, which prevents the TDCC with the true model from being 1.00. The analysis with PP_REG again includes two spurious variables, x_5 and x_9. It is possible that an adjustment to increase the degrees of freedom in a similar fashion to that for RP_REG is required to account for estimating the projections in PP_REG. The analysis with SRD/RCC also identifies x_1 and x_2 as the important variables in the correct order.

3.3 Nonmonotonic Relationships: $y_3 = f_3(x_1, x_2, \ldots, x_8)$

Result y_3 is severely nonlinear in behavior as illustrated in Fig. 3, which contains a plot of y_3 versus the two most important variables, x_1 and x_2. The true model summary in Table 3 indicates that x_1 and x_2 are responsible for most of the uncertainty (95%) in y_3; further, x_3 accounts for about an additional 3% and x_4 an additional 1% of the uncertainty in y_3. The analyses with LIN_REG and RANK_REG demonstrate that these methods are not capable of modeling this data. Both analyses result in models with no variables selected as important. Hence, both analyses result in R^2 values of 0.00. The analysis with PP_REG does a decent job of picking the two most important variables and giving reasonable estimates of their contribution to the uncertainty in y_3 but fails to identify the variables x_3 and x_4. The analysis with the SRD/RCC test also identifies the two most important variables correctly. The analyses with QUAD_REG and GAM do an even better job by picking out and ordering the four most important variables correctly with reasonably good R^2 estimates, although the R^2 estimates from GAM are closer to the true values than those from QUAD_REG. The analysis with RP_REG and LOESS both do an excellent job of accurately estimating the contribution of the three most important variables x_1 , x_2 and x_3, but fail to identify variable x_4. In this particular example, the standard regression tree defined in Eqs. (3.42) and (3.43) of Ref. 1 (results not displayed) gives sequential R^2 estimates of 0.72, 0.92, and 0.90 as x_1, x_2 and x_3 enter the model. For RP_REG, these values are 0.72, 0.97, and 0.98, which are closer to the true values. In addition, the RP_REG procedure provided superior results to the standard regression tree approach in most of the other examples considered in this presentation.

3.4 Nonmonotonic Relationship: $y_4 = f_4(x_1, x_2, x_3)$

Result y_4 is the most difficult outcome to analyze for all of the regression methods. As shown in Table 4, the linear methods (i.e., LIN_REG, RANK_REG and QUAD_REG) have an R^2 below 0.2 The analysis with QUAD_REG fails because the sinusoidal relationship that can be seen in Fig. 4 departs too much from a quadratic. The oscillating behavior of y_4 is also difficult for LIN_REG and RANK_REG to model. The analysis with PP_REG, which often overfits the data, this time identified only x_2 and x_3 for inclusion in the model; the reasons for this are unclear. The analysis with GAM has an R^2 value of 0.79 and identifies the two most important variables correctly. However, GAM also includes the spurious variable x_4. The analysis with LOESS was the most successful on this example. It has an R^2 value of 0.95 and identifies the three important inputs correctly. The analysis with RP_REG has an R^2 value of 0.90, and also identifies all three important inputs correctly. Both LOESS and RP_REG give reasonable estimates of the R^2 contribution of each variable as well. The analysis with the SRD/RCC test also identifies x_2 and x_1 as the two most important variables in the correct order but fails to identify x_3 and includes x_6 spuriously.

4. Example Results: Two-Phase Fluid Flow

The regression-based sensitivity analysis procedures are now illustrated with results from an uncertainty/sensitivity analysis of a model for two phase fluid flow[12-14] carried out as part of the 1996 compliance certification application (CCA) for the Waste Isolation Pilot Plant (WIPP).[4, 5] The CCA involved nX = 57 uncertain variables,[22] with 31 of these variables used in the two-phase fluid flow analysis considered in this section (Table 5). The two-phase fluid flow analysis considered six different scenarios (i.e., modeling cases; see Table 6, Ref. 22) and generated several hundred time-dependent analysis results for each modeling case (e.g., see Table 1, Ref. 13, for a partial listing of these results). A small subset of these results is considered in this presentation. In particular, the modeling case corresponding to a drilling intrusion at 1000 yr that penetrates both the repository and an underlying region of pressurized brine is used as an example (i.e., an E1 intrusion at 1000 yr in the terminology of the 1996 WIPP CCA; see Table 6, Ref. 22), and three time-dependent analysis results are used for illustration (Table 6).

The example analysis used Latin hypercube sampling to generate a mapping between analysis inputs and analysis results of the form indicated in Eqs. (1.5) and (1.6) of Ref. 1. In particular, three replicated (i.e., independently generated) Latin hypercube samples[25, 26] of size nS = 100 were used. Thus, the analysis actually had three samples of the form indicated in Eq. (1.5) of Ref. 1 and three mappings of the form indicated in Eq. (1.6) of Ref. 1. This replication was performed to provide a way to test the stability (i.e., reproducibility) of analysis results (Sect. 7, Ref. 22). For convenience, the individual replicates are referred to as replicate R1, R2 and R3, respectively. The 100 time-dependent values for the variables indicated in Table 6 (i.e., *BRNREPTC*, *REP_SATB*, *WAS_PRES*) that result for replicate R1 are shown in Fig. 5.

The three time-dependent results indicated in Table 6 are analyzed at 1000 yr and 10,000 yr. The results at 1000 yr are for undisturbed conditions immediately prior to the drilling intrusion at 1000 yr. Because of this timing, the 1000 yr results are unaffected by the drilling intrusion and thus are very different from the 10,000 yr results.

4.1 Cumulative Brine Flow at 1000 yr (*BRNREPTC.1K*)

All of the analysis methods perform well for *BRNREPTC.1K* (Table 7), with all methods identifying *HALPOR* as the most important variable and all the regression-based methods identifying *HALPOR*, *WMICDFLG*, *ANHPRM* and *HALPRM* as the four most important variables. Specifically, all regression-based methods indicate that *HAL-*

POR accounts for approximately 96% of the uncertainty in *BRNREPTC.1K* and that the four most important variables collectively account for between 98% and 99% of the uncertainty in *BRNREPTC.1K*. The examination of scatterplots shows the dominant effect of *HALPOR* and also the more subtle effects associated with *WMICDFLG*, *ANHPRM* and *HALPRM* (Fig. 6). The similarity of the results obtained with LIN_REG and RANK_REG indicates that the relationships between *BRNREPTC.1K* and the sampled variables affecting *BRNREPTC.1K* are effectively linear. In this situation, all of the regression-based methods are producing models of similar predictive capability. However, as suggested by the incremental changes in the number of degrees of freedom, the nonparametric regression procedures (i.e., LOESS, PP_REG, RP_REG, GAM) are producing models that are more complicated than those produced by the parametric regression procedures (i.e., LIN_REG, RANK_REG, QUAD_REG). For PP_REG and RP_REG, the negative value for the incremental degrees of freedom associated with the addition of *HALPRM* and *WASTWICK* to the respective models indicates a reduction in complexity for the constructed model with the addition of this variable.

It is likely that some of the variables added near the ends of the stepwise procedures for the individual regression procedures are spurious. For example, the variable *BHPRM* added at the end of the analysis with PP_REG is obviously spurious because *BHPRM* does not affect *BRNREPTC.1K*. With approximately 30 uncertain variables under consideration and use of an α-value cutoff of 0.02, the selection of spurious variables near the end of a stepwise analysis is always a possibility.

The decreasing PRESS values for the LIN_REG, RANK_REG, QUAD_REG, and GAM indicate that the data is not being overfitted. However, there are some jumps in the PRESS values for LOESS, PP_REG and RP_REG as variables with small indicated effects are added to the regression model, which suggests that some overfitting of the data is taking place. Further, with the exception of PP_REG, the values for the TDCC (i.e., C_T) range from 0.92 to 0.96 for the individual regression procedures and indicate a high degree of reproducibility for results obtained with the three replicated LHSs of size 100. The PP_REG procedure has a lower level of reproducibility as indicated by a TDCC of 0.81.

The SRD/RCC test identifies the dominant effect associated with *HALPOR* but misses the smaller effects associated with *WMICDFLG*, *ANHPRM* and *HALPRM*.

4.2 Cumulative Brine Flow at 10,000 yr (*BRNREPTC.10K*)

For *BRNREPTC.10K*, the methods generally agree on the three most important variables (i.e., *BHPRM*, *BPCOMP*, *HALPOR*) but there is some inconsistency with respect to the fourth most important variable (Table 8). The methods also do not agree on the total amount of uncertainty that can be explained. As shown by the scatterplots of the four most important input variables (Fig. 7), there is a definite monotonic relationship between these variables and *BRNREPTC.10K*. The linear methods LIN_REG and RANK_REG each have a relatively low final R^2

value of 0.71. In addition, GAM has a final R^2 value of 0.79, which suggests that in addition to nonlinearity there is also interaction between input variables. The remaining methods, QUAD_REG, LOESS, PP_REG, and RP_REG, all have R^2 values of about 0.8 or higher after inclusion of the fifth most important variable. After that, there is considerable disagreement on which inputs make additional contributions to the uncertainty in *BRNREPTC.10K*. Thus, the only safe inference that can be drawn from the collective analyses is that these first five inputs (i.e., *BHPRM*, *BPCOMP*, *HALPOR, WMICDFLG,* and *ANHPRM*) are giving rise to about 80 – 90% of the uncertainty in *BRNREPTC.10K*. For the PP_REG and RP_REG, increases in PRESS values near the end of the stepwise process indicate that overfitting of the data may be taking place as variables with small effects are added to the models.

The SRD/RCC test agrees with the regression methods on four of the first five variables but also includes *BPPRM* as the fifth most important input, which is not in any of the other models except RP_REG. This difference probably results from the −0.75 rank correlation between *BPPRM* and *BPCOMP* (see Table 5). All the regression-based methods select *BPCOMP* as the second variable in the stepwise procedure. Because of the indicated correlation, the resultant regression model includes effects that derive from both *BPCOMP* and *BPPRM*, which reduces the likelihood that *BPPRM* will be selected at a later step. In contrast, the SRD/RCC test examines the effects of variables individually, which makes it more effective in identifying the effects of correlated variables than is the case for stepwise regression procedures.

The PP_REG procedure has a very low reproducibility with a TDCC value of 0.40. The LOESS and RP_REG procedures also have relatively low TDCC values of 0.72 and 0.71, respectively. In contrast, the TDCC values for the other methods range between 0.87 and 0.96, which indicates fairly high levels of reproducibility.

4.3 Brine Saturation at 1000 yr (*REP_SATB.1K*)

The analyses for *REP_SATB.1K* (Table 9) produce results very similar to those *BRNREPTC.1K* (Table 7), where the linear methods performed well. All the methods agree on the four most important input variables (i.e., *HALPOR*, *WGRCOR*, *WMICDFLG*, *WASTWICK*). All the regression-based methods indicate that *HALPOR* accounts for about 60% of the uncertainty in *REP_SATB.1K*. They also indicate that *WGRCOR* is responsible for an additional 20% of the uncertainty in *REP_SATB.1K*. The dominant effects of *HALPOR* and *WGRCOR* are clearly evident in the corresponding scatterplots in Fig. 8. In addition, *WMICDFLG* and *WASTWICK* account for about another 10% and 5%, respectively, of the uncertainty in *REP_SATB.1K*. The SRD/RCC test also identifies these four variables in the same order as the regression-based methods. All methods also have high TDCC values, indicating a high level of reproducibility. However, PP_REG and RP_REG have jumps in PRESS values at the end of the stepwise process as variables with very small effects are added to the models, which indicates that an overfitting of the data may be taking place.

4.4 Brine Saturation at 10,000 yr (*REP_SATB.10K*)

All methods identify *WGRCOR* and *BHPRM* as the two most important contributors to the uncertainty in *REP_SATB.10K* (Table 10). The linear methods (i.e., LIN_REG and RANK_REG) underperform the other regression methods in that they appear to underestimate the contributions of *WGRCOR* and *BHPRM* to the uncertainty in *REP_SATB.10K* (i.e., compare R^2 values for the different regression procedures in Table 10). Specifically, LIN_REG and RANK_REG indicate that *WGRCOR* accounts for about 22 – 28% of the uncertainty in *REP_SATB.10K* while the other methods indicate that *WGRCOR* contributes in the range of 42 – 48% of the uncertainty in *REP_SATB.10K*. From this, it is then clear that *BHPRM* accounts for another 15 – 20% of the uncertainty above and beyond that accounted for by *WGRCOR*.

After *WGRCOR* and *BHPRM*, the individual analyses generally indicate that additional contributions to the uncertainty in *REP_SATB.10K* are made primarily by *HALPOR* (~10 – 15%) and *BPCOMP* (~5%), with smaller contributions from *WMICDFLG*, *ANHPRM* and *WASTWICK* (~ 2% each). As shown by the scatterplots in Fig. 9, *WGRCOR* and *BHPRM* have visually discernable effects on *REP_SATB.10K*, while the less important contributors to the uncertainty in *REP_SATB.10K* have effects that are identifiable by the analysis procedures but are less apparent in a visual examination.

Although PP_REG has a reasonably high R^2 value, it has a low TDCC of 0.62. The reasons for the lack of reproducibility, and thus overall poor performance of the PP_REG procedure in this example, are not clear at this time. Also, PP_REG and RP_REG again have jumps in PRESS values at the end of the stepwise process as variables with very small effects are added to the models, which indicates that an overfitting of the data may be taking place.

The other regression methods have TDCCs between 0.83 and 0.92, which suggests that they are providing more reproducible results than the PP_REG procedure. The SRD/RCC test agrees with the regression methods on the first four variables and also has a high TDCC of 0.93. It also includes *BPPRM* when none of the other methods do. As discussed in conjunction with *BRNREPTC.10K* in Sect. 4.2, this difference in variable selection probably results from the −0.75 rank correlation between *BPPRM* and *BPCOMP*.

4.5 Pressure at 1000 yr (*WAS_PRES.1K*)

The analyses for *WAS_PRES.1K* (Table 11) show again that linear models can work quite well in some situations. The dominant variable contributing to the uncertainty in *WAS_PRES.1K* is *WMICDFLG*, with the regression methods indicating that *WMICDFLG* accounts for approximately 85% of the uncertainty in *WAS_PRES.1K*. After *WMICDFLG*, the variable *WGRCOR* contributes an additional 10% of the uncertainty to *WAS_PRES.1K*. Owing to the linearity of the relationships between *WMICDFLG*, *WGRCOR* and *WAS_PRES.1K* (Fig. 10), the estimated contributions of *WMICDFLG* and *WGRCOR* to the uncertainty in *WAS_PRES.1K* are approximately the same for all regression methods. Further, the next two most important contributors to the uncertainty in *WAS_PRES.1K* (i.e., *WASTWICK* and *HALPOR*) are also consistently identified by all the regression methods. However, the effects of *WASTWICK* and *HALPOR* are small relative to the effects associated with *WMICDFLG* and *WGRCOR* as indicated by the incremental R^2 values associated with individual regressions and the scatterplots in Fig. 10. As indicated by the incremental degrees of freedom for individual regression models, the nonparametric regression models are considerably more complex than the models constructed with the linear regression procedures.

The SRD/RCC test produces results consistent with the regression methods in that it identifies *WMICDFLG*, *WGRCOR* and *WASTWICK*, in that order, as the three dominant contributors to the uncertainty in *WAS_PRES.1K*. However, the identification of an effect for *SHPRMASP* by the SRD/RCC test is probably spurious.

All of the procedures result in TDCCs close to or above 0.9. Thus, reproducible results for all procedures are being obtained for the dominant contributors to the uncertainty in *WAS_PRES.1K*. However, the large number of variables with marginal effects selected at the end of the analysis with PP_REG and the associated increases in PRESS values suggests that an overfitting of the data is taking place. Some increases in PRESS values near the end of the stepwise process also takes place for LOESS and RP_REG.

4.6 Pressure at 10,000 yr (*WAS_PRES.10K*)

The limitations of linear methods for sensitivity analysis are shown in the analyses for *WAS_PRES.10K* (Table 12). The dominant variable contributing to the uncertainty in *WAS_PRES.10K* is *BHPRM* (Fig. 11) and provided the illustrative example used for scatterplot smoothers in Sect. 3.1 of Ref. 1. The relationship between *BHPRM* and *WAS_PRES.10K* is both nonlinear and nonmonotonic. Linear regression with raw or rank-transformed data is essentially useless in this case and fails to even include *BHPRM* in the model when it is clearly the input most responsible for the uncertainty in the output (Table 12). While linear regression with raw or rank-transformed data had final R^2 values of about 0.27, the nonparametric methods and also QUAD_REG had final R^2 values in the 0.8 – 0.9 range. Because of its limitations in higher dimensions, LOESS will sometimes include too few variables in the model, which may be the case here.

The analyses with QUAD_REG, LOESS, GAM, PP_REG and RP_REG all had reasonably high R^2 values (i.e., 0.85, 0.84, 0.79, 0.83, 0.95), and generally agreed on the four most important variables (i.e., *BHPRM*, *HALPRM*, *BPCOMP*, *ANHPRM*), although RP_REG and PP_REG include *WGRCOR* as the second and third variable, respectively, in the model (see Table 12). All methods indicated that *BHPRM* was responsible for about 50% of the uncertainty in *WAS_PRES.10K*. However, PP_REG had a TDCC of 0.64, which is low. The analysis with RP_REG has a high R^2 value of 0.95 and a TDCC of 0.86. The analyses with GAM and QUAD_REG have TDCC values of 0.75 and 0.86, respectively, but have lower R^2 values than RP_REG. Based on the methods with high R^2 values, a breakdown for percentage contributors to the uncertainty in *WAS_PRES.10K* would be *BHPRM* with 50%, *BPCOMP* with about 10%, *HALPRM* with 5 – 10%, WGRCOR with 5 – 10%, and *ANHPRM* with 5 – 10%. After that, *HALPOR* may account for as much as another 5%. Again, the SRD/RCC test agrees with the regression methods on the first four variables and has a high TDCC of 0.91.

As seen in other analyses, jumps in PRESS values occur for LOESS, PP_REG and RP_REG near the end of the stepwise process.

5. Observations and Insights

The following observations and insights are based on the examples described in this presentation. Nonparametric methods worked quite well for sensitivity analysis and provide a useful addition to currently employed sampling-based sensitivity analysis procedures.

The overall best method considered in this study is RP_REG. In the test cases, it almost always ordered the input variables correctly and estimated the contributions to R^2 accurately. The drawback is that it generally takes longer to apply than any of the other methods.

The GAM and QUAD_REG procedures displayed good performance on the test data and are fast computationally. The QUAD_REG procedure can model a certain degree of interaction while GAM does not. However, GAM can model more general nonlinearity than QUAD_REG. Also, multiplicative interaction terms could be used in GAM to make it a more general method.

The LOESS and PP_REG procedures exhibited some problems that could reduce their usefulness for sensitivity analysis. Specifically, LOESS sometimes failed to identify important input variables, although it usually identified the two most important variables. The PP_REG procedure showed a tendency to err in the opposite direction and often included insignificant input variables in the model. The tendency was indicted by the jumps in PRESS values that often occurred near the end of the stepwise implementation of PP_REG.

The SRD/RCC test also performed well and identified the dominant variables in all the analyses. The drawback to this test is that it does not provide the fraction of the uncertainty in the dependent variable explained by each of the identified independent variables. However, it has an advantage over the non-parametric regression procedures in being both conceptually simple and computationally quick.

Given the nonlinear relationships that can be present in analyses with complex computer models, one should be cautious about using only linear methods for sensitivity analysis. However, when a linear regression with raw or rank-transformed data is appropriate, it should be used as it is the easiest method to implement and interpret.

A reasonable analysis strategy is initially to fit linear regressions with raw and rank-transformed data and observe the R^2 values. If these values are below 0.9, then fit a QUAD_REG surface. If QUAD_REG also has an R^2 below 0.9, then fit a GAM surface. If the GAM surface still has a low R^2, then fit a RP_REG model. This approach restricts the use of the more computationally demanding RP_REG procedure to situations where its use is necessary. This is important because real analyses can involve carrying out sensitivity analyses for hundreds of time-dependent analysis results (e.g., see the sensitivity analyses summarized in Ref. 4).

If the resources are not available to carry out the indicated sequence of nonparametric regressions, then the SRD/RCC test provides a computationally efficient way to identify nonlinear relationships. Another analysis possibility is to use the SRD/RCC test to identify the dominant contributors to the uncertainty in a dependent variable, and then consider only these dominant variables in a nonparametric regression analysis.

The authors' experience is that linear regression with rank-transformed data and examination of associated scatterplots are usually sufficient to carry out a successful sensitivity analysis. However, there are situations where this approach will not be successful. Then, nonparametric regression procedures can often provide the needed techniques to determine the relationships between uncertain analysis inputs and analysis results.

Additional generalized regression procedures also exist that merit investigation for their potential usefulness in sensitivity analysis. For example, additional procedures for additive modeling include the Alternating Conditional Expectation (ACE) algorithm[27] and the Additivity and Variance Stabilization (AVAS) algorithm[28] (see Ref. 29, pp. 175 – 194, for additional discussion of the ACE and AVAS algorithms). There are also more sophisticated forms of recursive partitioning such as Multivariate Adaptive Regression Splines (MARS) (Ref. 30; also Ref. 29, pp. 275 – 277) and Smoothed and Unsmoothed Piecewise-Polynomial Regression Trees (SUPPORT).[31] As the recursive partitioning technique (Sect. 3.3.4, Ref. 1) was the best of the presented nonparametric regression methods, these two techniques merit investigation for use in sensitivity analysis. Gaussian process models have also been proposed for use in sensitivity analysis.[32-34] A comparison of the performance of Gaussian process models and nonparametric regression models in sensitivity analysis would be interesting.

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References

1. Storlie, C.B. and J.C. Helton. To Appear. "Multiple Predictor Smoothing Methods for Sensitivity Analysis: Description of Techniques," *Reliability Engineering and System Safety*.

2. Saltelli, A., K. Chan, and E.M. Scott (eds). 2000. *Sensitivity Analysis*. New York, NY: Wiley.

3. Campolongo, F., A. Saltelli, T. Sorensen, and S. Tarantola. 2000. "Hitchhiker's Guide to Sensitivity Analysis," *Sensitivity Analysis*. Ed. A. Saltelli, K. Chan, and M. Scott. New York, NY: John Wiley & Sons.

4. Helton, J.C. and M.G. Marietta. 2000. "Special Issue: The 1996 Performance Assessment for the Waste Isolation Pilot Plant," *Reliability Engineering and System Safety*. Vol. 69, no. 1-3, pp. 1-451.

5. Helton, J.C., D.R. Anderson, H.-N. Jow, M.G. Marietta, and G. Basabilvazo. 1999. "Performance Assessment in Support of the 1996 Compliance Certification Application for the Waste Isolation Pilot Plant," *Risk Analysis*. Vol. 19, no. 5, pp. 959 - 986.

6. Draper, N.R. and H. Smith. 1981. *Applied Regression Analysis*. 2nd ed. New York, NY: John Wiley & Sons.

7. Helton, J.C., F.J. Davis, and J.D. Johnson. 2005. "A Comparison of Uncertainty and Sensitivity Analysis Results Obtained with Random and Latin Hypercube Sampling," *Reliability Engineering and System Safety*. Vol. 89, no. 3, pp. 305-330.

8. Iman, R.L. and W.J. Conover. 1987. "A Measure of Top-Down Correlation," *Technometrics*. Vol. 29, no. 3, pp. 351-357.

9. Hora, S.C. and J.C. Helton. 2003. "A Distribution-Free Test for the Relationship Between Model Input and Output when Using Latin Hypercube Sampling," *Reliability Engineering and System Safety*. Vol. 79, no. 3, pp. 333-339.

10. Conover, W.J. 1980. *Practical Nonparametric Statistics*. 2nd ed. New York, NY: John Wiley & Sons.

11. Helton, J.C. and F.J. Davis. 2002. "Illustration of Sampling-Based Methods for Uncertainty and Sensitivity Analysis," *Risk Analysis*. Vol. 22, no. 3, pp. 591-622.

12. Vaughn, P., J.E. Bean, J.C. Helton, M.E. Lord, R.J. MacKinnon, and J.D. Schreiber. 2000. "Representation of Two-Phase Flow in the Vicinity of the Repository in the 1996 Performance Assessment for the Waste Isolation Pilot Plant," *Reliability Engineering and System Safety*. Vol. 69, no. 1-3, pp. 205-226.

13. Helton, J.C., J.E. Bean, K. Economy, J.W. Garner, R.J. MacKinnon, J. Miller, J.D. Schreiber, and P. Vaughn. 2000. "Uncertainty and Sensitivity Analysis for Two-Phase Flow in the Vicinity of the Repository in the 1996 Performance Assessment for the Waste Isolation Pilot Plant: Undisturbed Conditions," *Reliability Engineering and System Safety*. Vol. 69, no. 1-3, pp. 227-261.

14. Helton, J.C., J.E. Bean, K. Economy, J.W. Garner, R.J. MacKinnon, J. Miller, J.D. Schreiber, and P. Vaughn. 2000. "Uncertainty and Sensitivity Analysis for Two-Phase Flow in the Vicinity of the Repository in the 1996 Performance Assessment for the Waste Isolation Pilot Plant: Disturbed Conditions," *Reliability Engineering and System Safety*. Vol. 69, no. 1-3, pp. 263-304.

15. Chan, K., S. Tarantola, and A. Saltelli. 2000. "Variance-Based Methods," *Sensitivity Analysis*. Ed. A. Saltelli, K. Chan, and E.M.S. Scott. New York, NY: Wiley. 167-197.

16. Li, G., C. Rosenthal, and H. Rabitz. 2001. "High-Dimensional Model Representations," *The Journal of Physical Chemistry*. Vol. 105, no. 33, pp. 7765-7777.

17. Rabitz, H. and O.F. Alis. 1999. "General Foundations of High-Dimensional Model Representations," *Journal of Mathematical Chemistry*. Vol. 25, no. 2-3, pp. 197-233.

18. Saltelli, A., S. Tarantola, and K.P.-S. Chan. 1999. "A Quantitative Model-Independent Method for Global Sensitivity Analysis of Model Output," *Technometrics*. Vol. 41, no. 1, pp. 39-56.

19. Sobol', I.M. 1993. "Sensitivity Estimates for Nonlinear Mathematical Models," *Mathematical Modeling & Computational Experiment*. Vol. 1, no. 4, pp. 407-414.

20. Yao, Q. and H. Tong. 2000. "Nonparametric Estimation of Ratios of Noise to Signal in Stochastic Regression," *Statistica Sinica*. Vol. 10, pp. 751-770.

21. Doskum, K. and A. Samaroz. 1995. "Nonparametric Estimation of Global Functionals and a Measure of the Explanatory Power of Covariates in Regression," *Annals of Statistics*. Vol. 23, no. 5, pp. 1443-1473.

22. Helton, J.C., M.-A. Martell, and M.S. Tierney. 2000. "Characterization of Subjective Uncertainty in the 1996 Performance Assessment for the Waste Isolation Pilot Plant," *Reliability Engineering and System Safety*. Vol. 69, no. 1-3, pp. 191-204.

23. Iman, R.L. and W.J. Conover. 1982. "A Distribution-Free Approach to Inducing Rank Correlation Among Input Variables," *Communications in Statistics: Simulation and Computation*. Vol. B11, no. 3, pp. 311-334.

24. Iman, R.L. and J.M. Davenport. 1982. "Rank Correlation Plots for Use with Correlated Input Variables," *Communications in Statistics: Simulation and Computation*. Vol. B11, no. 3, pp. 335-360.

25. McKay, M.D., R.J. Beckman, and W.J. Conover. 1979. "A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code," *Technometrics*. Vol. 21, no. 2, pp. 239-245.

26. Helton, J.C. and F.J. Davis. 2003. "Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems," *Reliability Engineering and System Safety*. Vol. 81, no. 1, pp. 23-69.

27. Breiman, L. and J.H. Friedman. 1985. "Estimating Optimal Transformers for Multiple Regression and Correlation (with discussion)," *Journal of American Statistical Association*. Vol. 80, pp. 580-619.

28. Tibshirani, R. 1988. "Estimating Optimal Transformations for Regression via Additivity and Variance Stabilization," *Journal of American Statistical Association*. Vol. 83, pp. 394-405.

29. Hastie, T.J. and R.J. Tibshirani. 1990. *Generalized Additive Models*. London: Chapman & Hall.

30. Friedman, J.H. 1991. "Multivariate Adaptive Regression Splines (with discussion)," *The Annals of Statistics*. Vol. 19, no. 1, pp. 1-141.

31. Chaudhuri, P., M. Huang, W. Loh, and R. Yao. 1994. "Piecewise Polynomial Regression Trees," *Statistica Sinica*. Vol. 4, pp. 143-167.

32. O'Hagan, A. 2006. "Bayesian Analysis of Computer Code Outputs: A Tutorial," *Reliability Engineering and System Safety*. Vol. 91, no. 10-11, pp. 1290-1300.

33. Kennedy, M.C., C.W. Anderson, S. Conti, and A. O'Hagan. 2006. "Case Studies in Gaussian Process Modelling of Computer Codes," *Reliability Engineering and System Safety*. Vol. 91, no. 10-11, pp. 1301-1309.

34. Oakley, J.E. and A. O'Hagan. 2004. "Probabilistic Sensitivity Analysis of Complex Models: A Bayesian Approach," *Journal of The Royal Statistical Society*. Vol. B66, pp. 751-769.

Figure Captions

Fig. 1. Analytic test model $y_1 = f_1(x_1, x_2) = 5x_1 + (5x_2)^2$

Fig. 2. Analytic test model $y_2 = f_2(x_1, x_2) = (1.5x_2 - 0.5)^4/(1.5x_1 - 0.5)^2$.

Fig. 3. Analytic test model $y_3 = f_3(x_1, x_2, \ldots, x_8)$ (see Eq. (5.9)) with surface averaged over $x_3, x_4, \ldots, x_8$.

Fig. 4. Scatterplots for x_1, x_2 and x_3 for analytic test model $y_4 = f_4(x_1, x_2, x_3)$ (see Eq. (5.10)).

Fig. 5. Time-dependent two-phase fluid flow results obtained with replicate R1 for a drilling intrusion at 1000 yr that penetrates the repository and an underlying region of pressurized brine (i.e., an E1 intrusion at 1000 yr).

Fig. 6. Scatterplots for cumulative brine flow at 1000 yr into repository (*BRNREPTC.1K*) for undisturbed conditions.

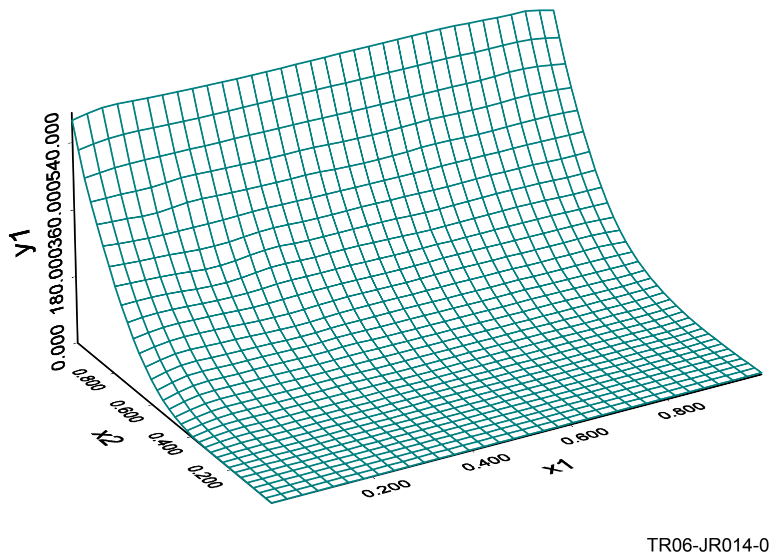
Fig. 7. Scatterplots for cumulative brine flow at 10,000 yr into repository (*BRNREPTC.10K*) for an E1 intrusion at 1000 yr.

Fig. 8. Scatterplots for average brine saturation at 1000 yr in waste panels not penetrated by a drilling intrusion (*REP_SATB.1K*) for undisturbed conditions.

Fig. 9. Scatterplots for average brine saturation at 10,000 yr in waste panels not penetrated by a drilling intrusion (*REP_SATB.10K)* for an E1 intrusion at 1000 yr.

Fig. 10. Scatterplots for pressure at 1000 yr in waste panel penetrated by a drilling intrusion (*WAS_PRES.1K*) for undisturbed conditions.

Fig. 11. Scatterplots for pressure at 10,000 yr in waste panel penetrated by a drilling intrusion (*WAS_PRES.10K*) for an E1 intrusion at 1000 yr.



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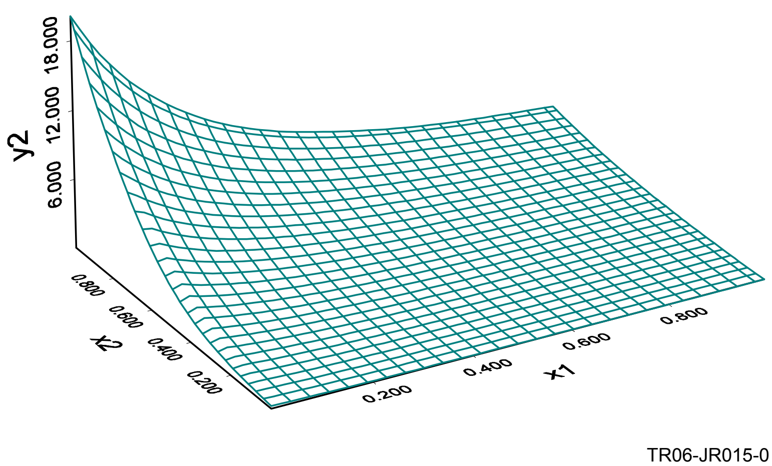

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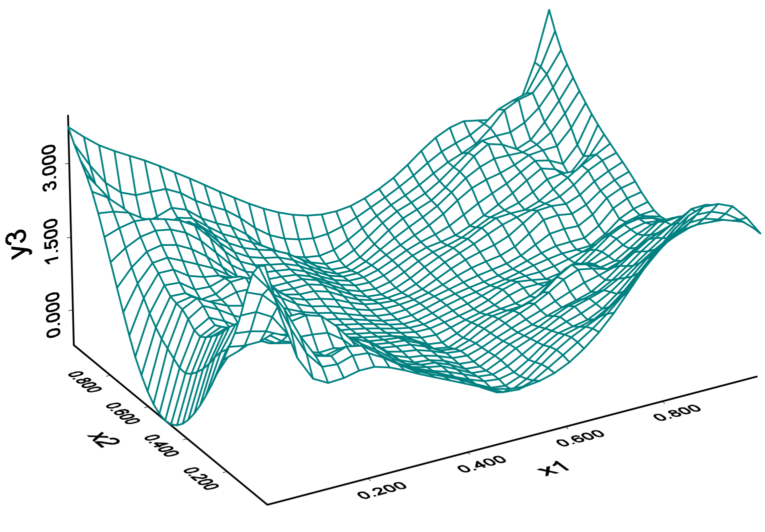
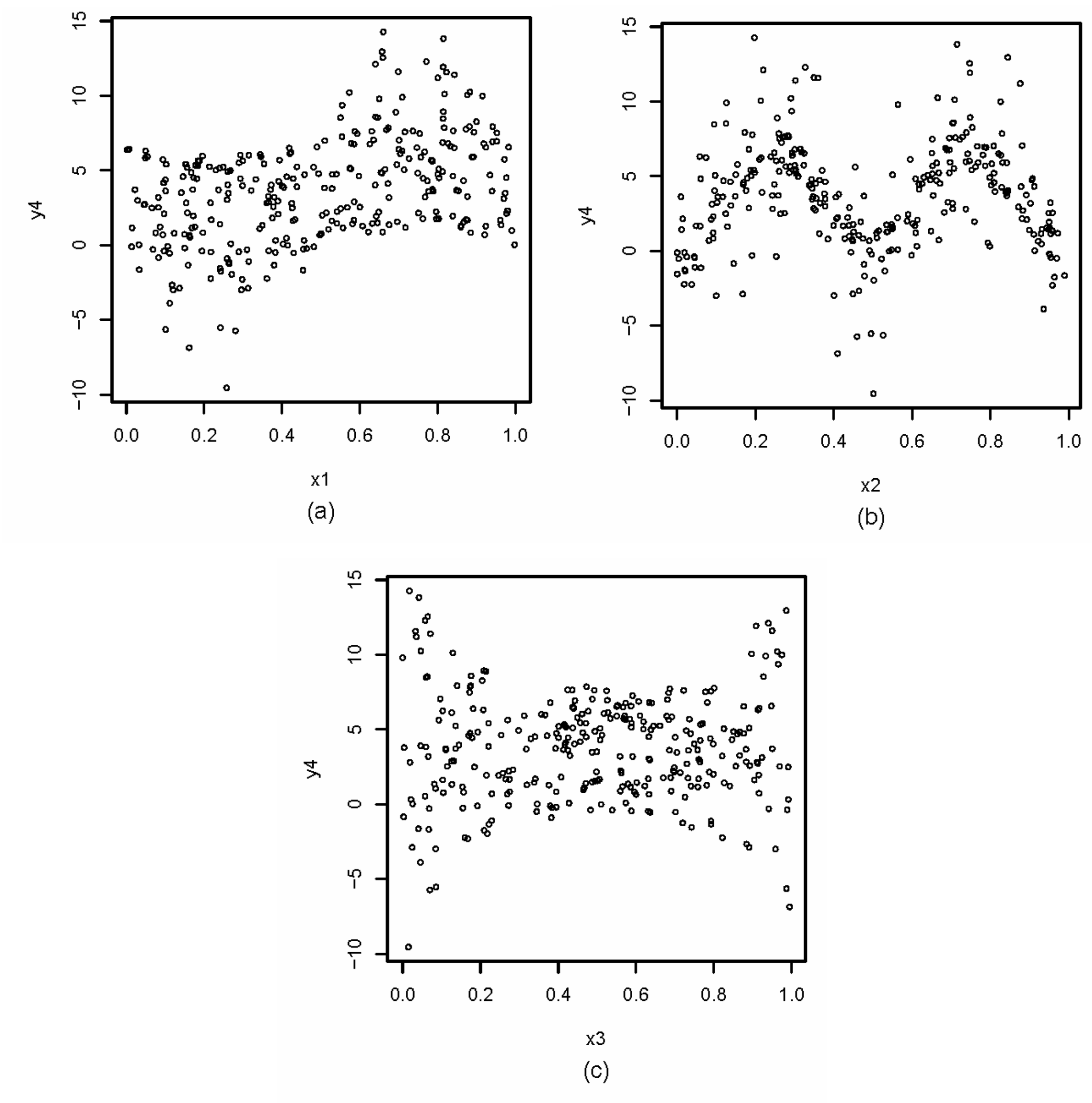


Fig. 3. Analytic test model $y_3 = f_3(x_1, x_2, \ldots, x_8)$ (see Eq. (5.9)) with surface averaged over $x_3, x_4, \ldots, x_8$.



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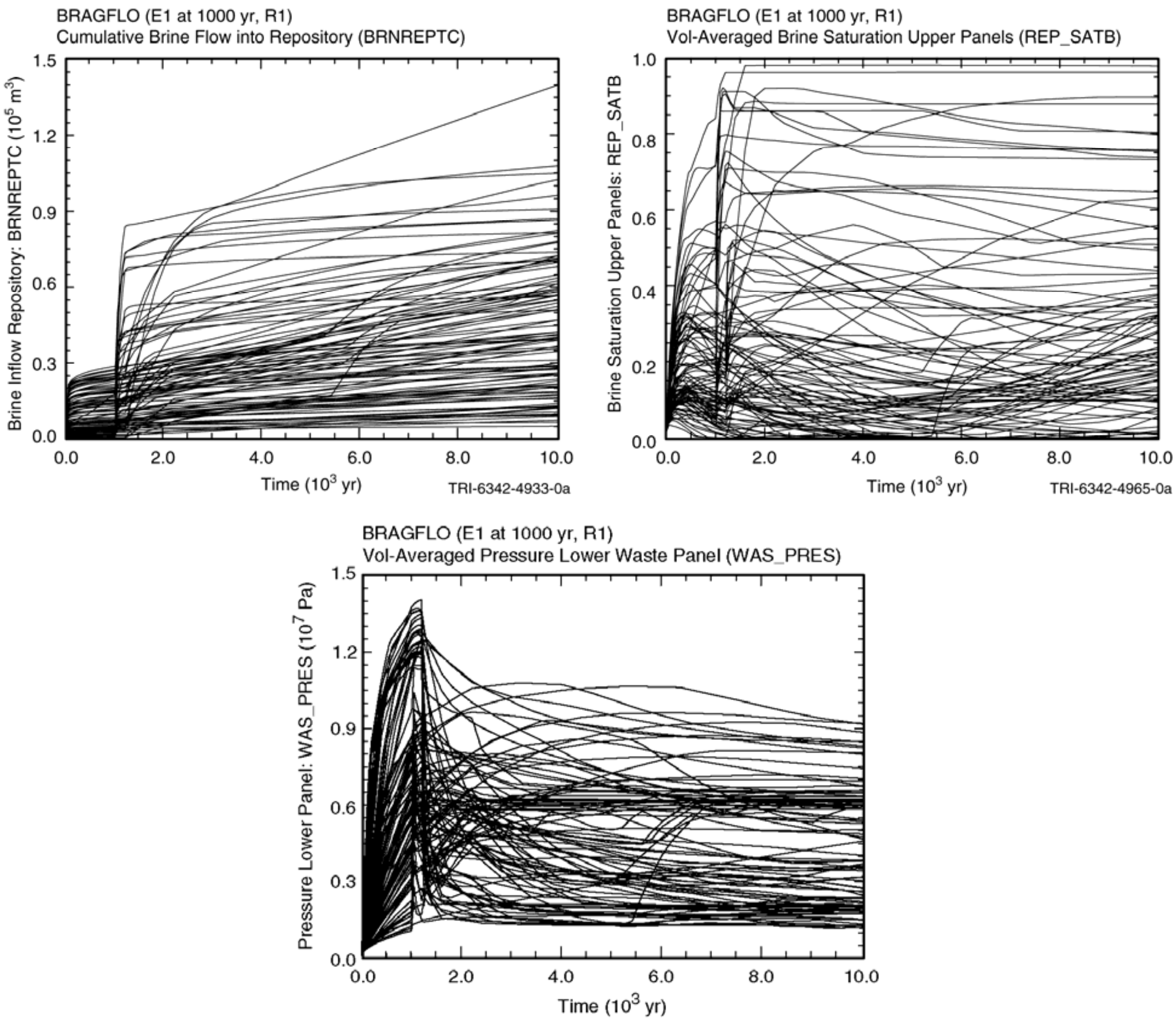

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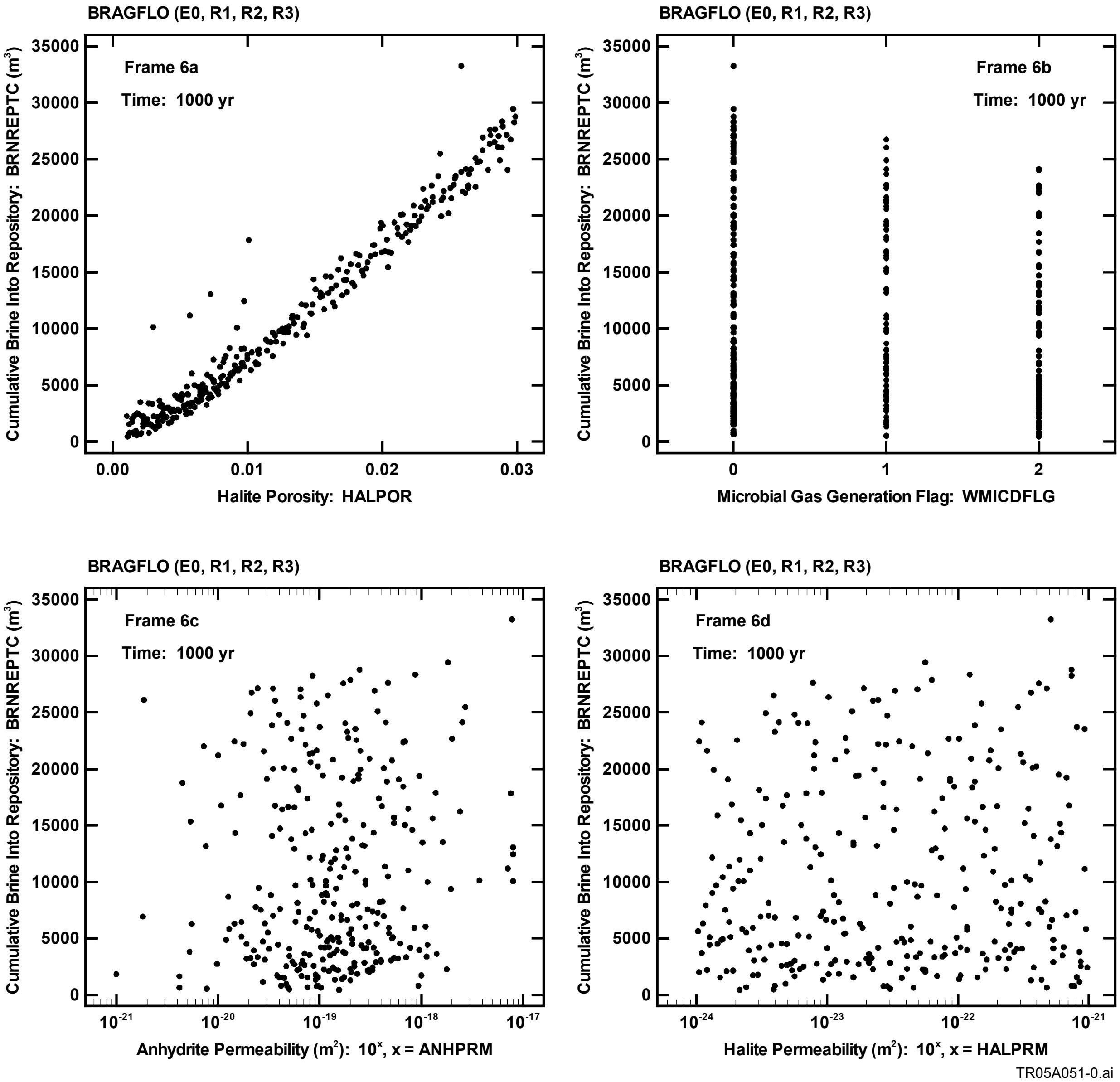

Fig. 6. Scatterplots for cumulative brine flow at 1000 yr into repository (*BRNREPTC.1K*) for undisturbed conditions.

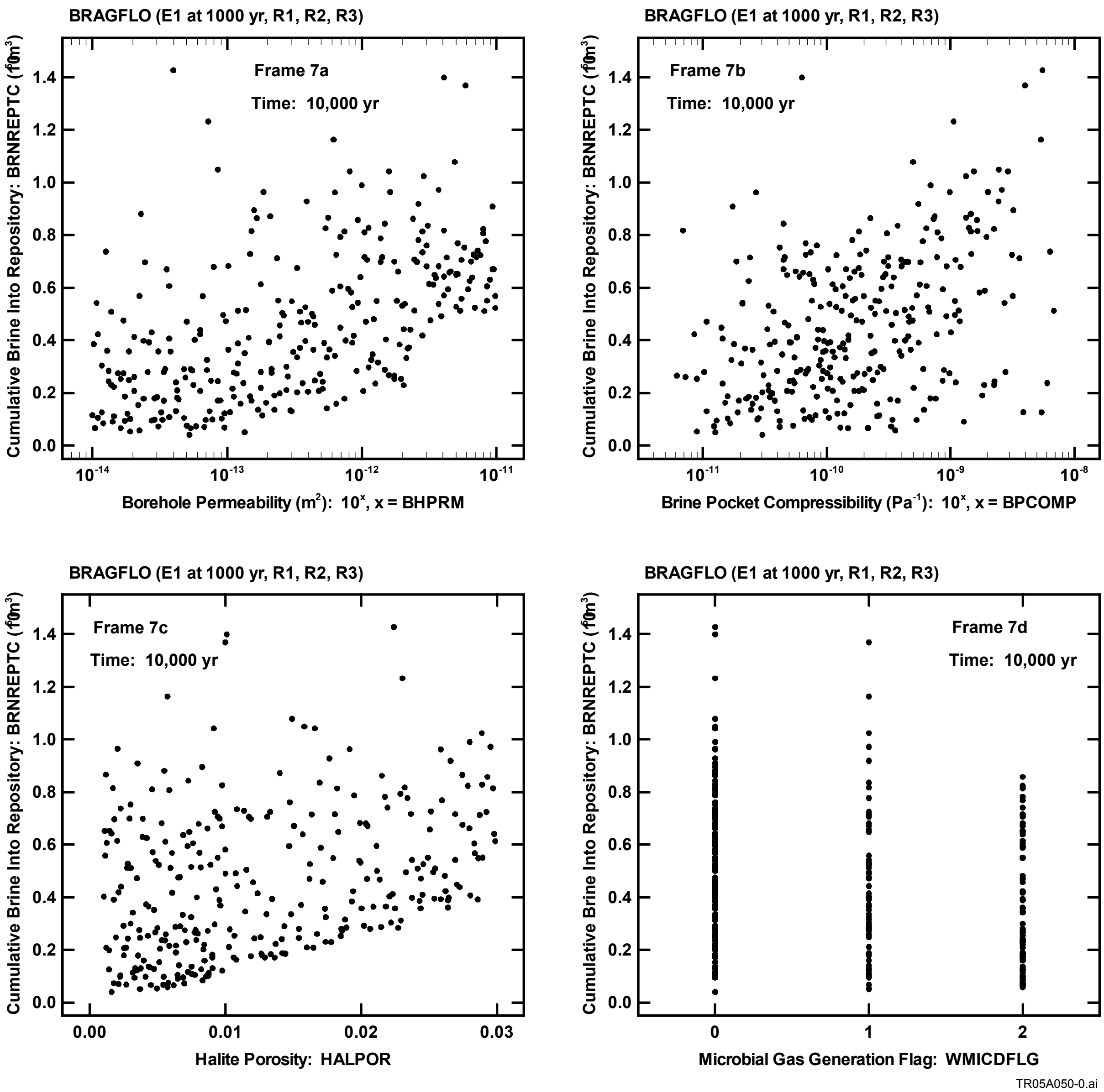

Fig. 7. Scatterplots for cumulative brine flow at 10,000 yr into repository (*BRNREPTC.10K*) for an E1 intrusion at 1000 yr.

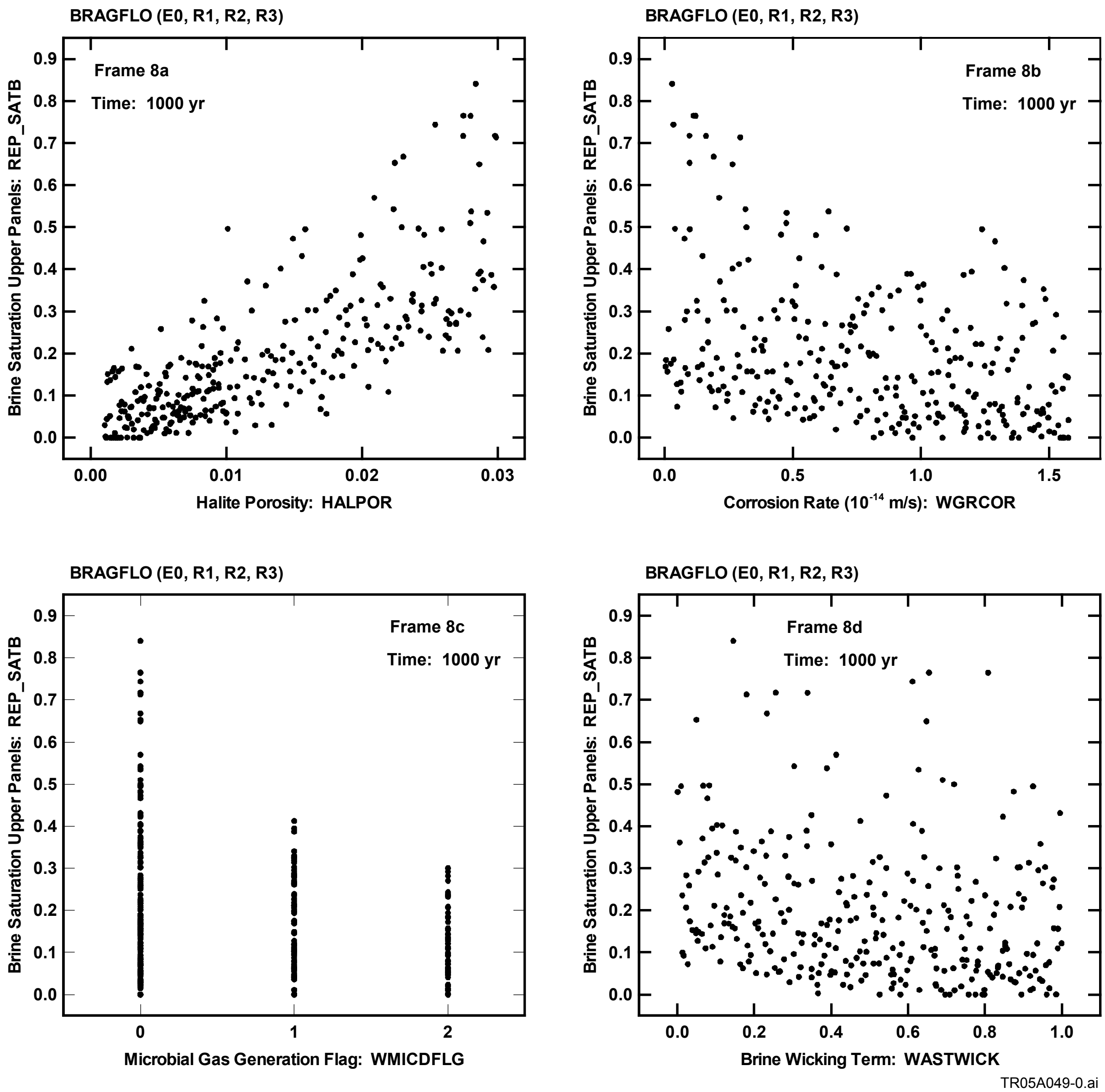

Fig. 8. Scatterplots for average brine saturation at 1000 yr in waste panels not penetrated by a drilling intrusion (*REP_SATB.1K*) for undisturbed conditions.

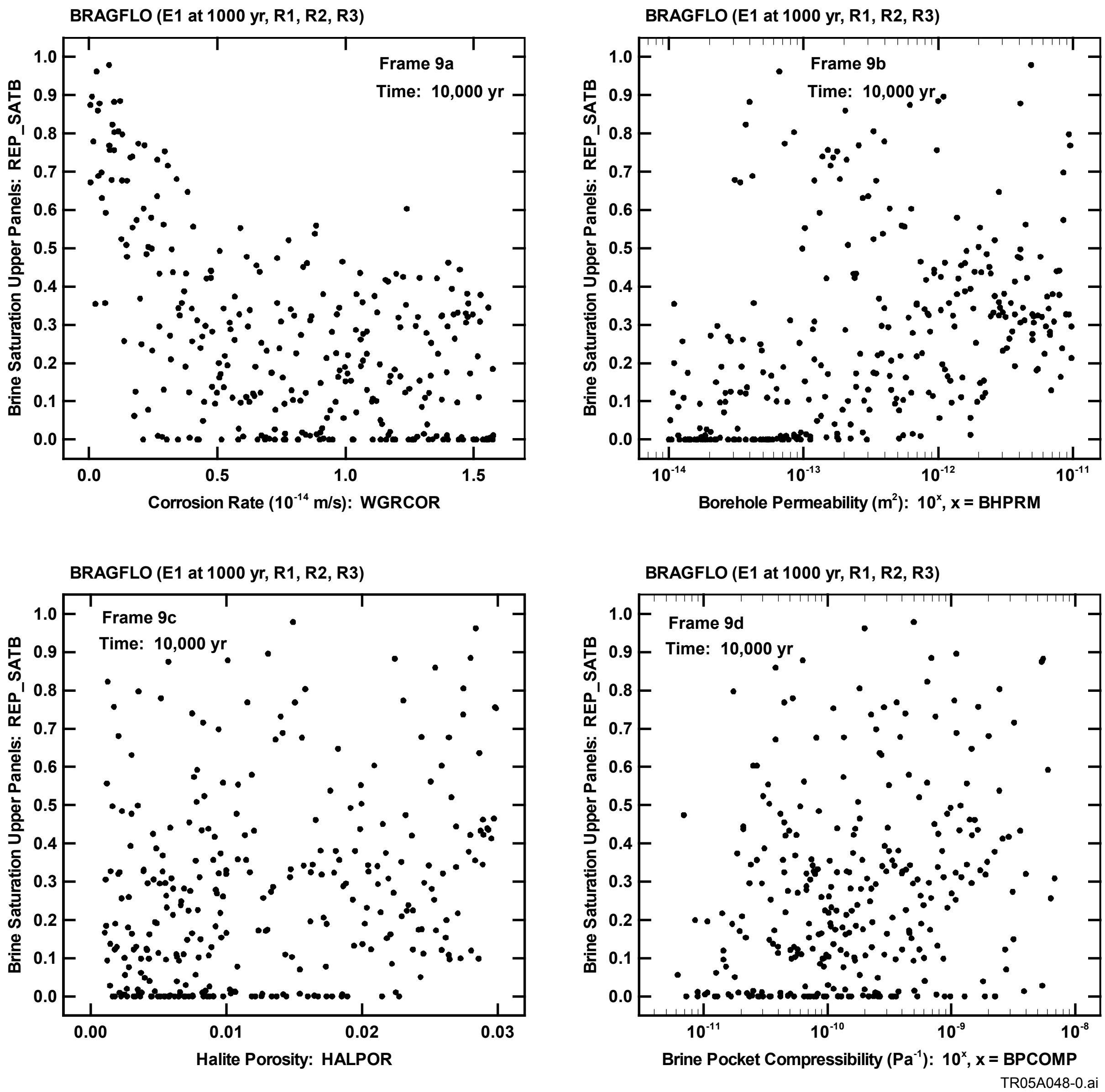

Fig. 9. Scatterplots for average brine saturation at 10,000 yr in waste panels not penetrated by a drilling intrusion (*REP_SATB.10K)* for an E1 intrusion at 1000 yr.

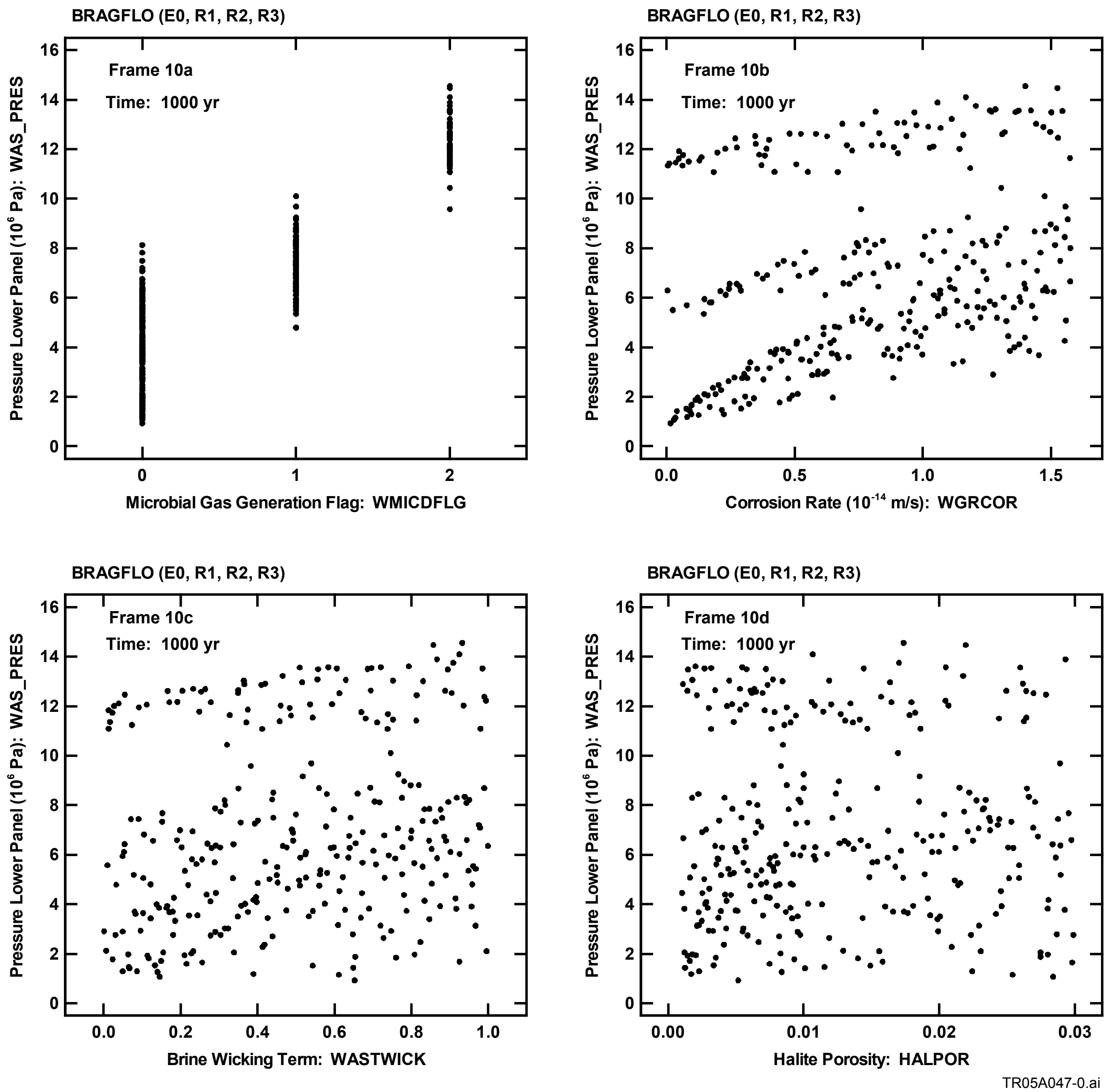

Fig. 10. Scatterplots for pressure at 1000 yr in waste panel penetrated by a drilling intrusion (*WAS_PRES.1K*) for undisturbed conditions.

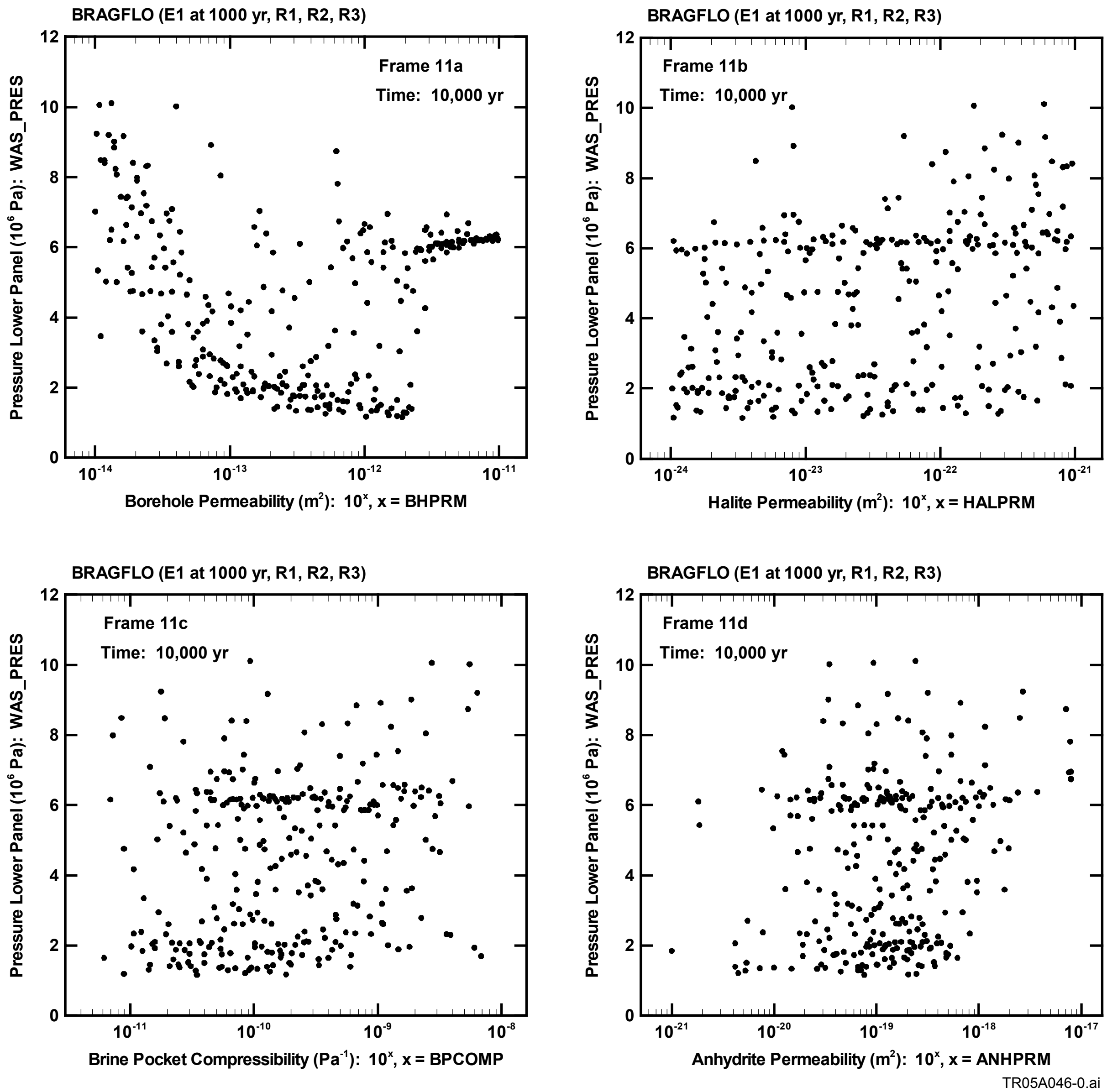

Fig. 11. Scatterplots for pressure at 10,000 yr in waste panel penetrated by a drilling intrusion (*WAS_PRES.10K*) for an E1 intrusion at 1000 yr.

Table 1. Sensitivity Analyses for Analytic Test Model $y_1 = f_1(x_1, x_2)$

Var[a]	$\boldsymbol{R^2}$[b]	***df***[c]	***p*-val**[d]	**PRS**[e]
LIN_REG				
x_2	0.7552	1.0	0.0000	1.87E6
R_A^2 = 0.7544[f], PRS_A = 1.86E6[g]				
C_T = 1.0000,[h] C_T w/true = 0.9294[i]				
LOESS				
x_2	0.9999	27.1	0.0000	6.74E2
R_A^2 = 0.9999, PRS_A = 6.79E2				
C_T = 1.0000, C_T w/true = 0.9294				
GAM				
x_2	0.9999	15.0	0.0000	6.80E2
x_1	1.0000	1.0	0.0000	7.55E1
R_A^2 = 1.0000, PRS_A = 4.50E1				
C_T = 1.0000, C_T w/true = 1.0000				

Var[a]	$\boldsymbol{R^2}$[b]	***df***[c]	***p*-val**[d]	**PRS**[e]
RANK_REG				
x_2	0.9774	1.0	0.0000	5.19E4
x_1	0.9842	1.0	0.0000	3.66E4
R_A^2 = 0.9841, PRS_A = 3.64E4				
C_T = 0.9744, C_T w/true = 1.0000				
PP_REG				
x_2	0.9999	13.2	0.0000	2.21E3
x_1	1.0000	14.4	0.0000	1.79E3
x_5	1.0000	25.3	0.0000	1.79E3
x_7	1.0000	–18.7	0.0009	1.79E3
R_A^2 = 1.0000, PRS_A = 2.00E0				
C_T = 0.9097, C_T w/true = 0.9453				
SRD/RCC TEST				
x_2	NA	4.0	0.0000	NA
x_1	NA	4.0	0.0101	NA
R_A^2 = NA, PRS_A = NA				
C_T = 0.9135, C_T w/true = 1.0000				

Var[a]	$\boldsymbol{R^2}$[b]	***df***[c]	***p*-val**[d]	**PRS**[e]
QUAD_REG				
x_2	0.9789	2.0	0.0000	1.63E5
R_A^2 = 0.9787, PRS_A = 1.62E5				
C_T = 1.0000, C_T w/true = 0.9294				
RP_REG				
x_2	0.9999	46.0	0.0000	7.63E2
x_1	1.0000	41.0	0.0000	5.06E1
R_A^2 = 1.0000, PRS_A = 4.01E1				
C_T = 1.0000, C_T w/true = 1.0000				
TRUE MODEL				
x_2	0.9999	NA[j]	NA	NA
x_1	1.0000	NA	NA	NA
R_A^2 = NA, PRS_A = NA				
C_T = NA, C_T w/true = 1.0000				

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[a] Variables listed in order of selection with sample of size nS = 300.

[b] Cumulative R^2 value with entry of each variable into model (see Eq. (3.7) for True Model and Eq. (3.6) for all other cases).

[c] Incremental degrees of freedom with entry of each variable into model for all cases except SRD/RCC test; *df* fixed at 4.0 for all variables for SRD/RCC test (see Eq. (2.6)).

[d] *p*-value for model with addition of each new variable (see Sect. 3.4 of Ref. 1 and related discussion for individual modeling cases).

[e] PRESS value for model with addition of each new variable (see Eq. (3.19), Ref. 1).

[f] Adjusted R^2 value for final model (see Eq. (2.1)).

[g] Adjusted PRESS value for final model (see Eqs. (3.22) and (3.25), Ref. 1).

[h] TDCC calculated between results for three replicated samples of size nS = 100 (see Eq. (2.2)).

[i] TDCC calculated between results obtained for case under consideration with a sample of size nS = 300 and the results obtained for the True Model (see Eq. (2.2)).

[j] NA indicates that result is not applicable.

Table 2. Sensitivity Analysis for Analytic Test Model $y_2 = f_2(x_1, x_2)$[a]

Var	R^2	*df*	*p*-val	**PRS**
LIN_REG				
x_2	0.4550	1.0	0.0000	1.11E3
x_1	0.6605	1.0	0.0000	7.03E2
R_A^2 = 0.6582, PRS_A = 6.94E2				
C_T = 1.0000, C_T w/true = 1.0000				
LOESS				
x_2	0.6199	27.1	0.0000	1.06E3
x_1	0.9995	45.7	0.0000	2.13E0
R_A^2 = 0.9993, PRS_A = 1.88E0				
C_T = 1.0000, C_T w/true = 1.0000				
GAM				
x_2	0.5340	4.0	0.0000	9.79E2
x_1	0.8046	15.0	0.0000	4.81E2
x_3	0.8225	10.0	0.0033	4.64E2
R_A^2 = 0.8034, PRS_A = 4.39E2				
C_T = 0.9460, C_T w/true = .9712				

Var	R^2	*df*	*p*-val	**PRS**
RANK_REG				
x_2	0.8013	1.0	0.0000	4.52E5
x_1	0.9784	1.0	0.0000	4.99E4
R_A^2 = 0.9783, PRS_A = 4.95E4				
C_T = 1.0000, C_T w/true = 1.0000				
PP_REG				
x_2	0.5323	3.0	0.0000	9.84E2
x_1	0.9994	32.5	0.0000	5.08E0
x_5	0.9999	4.6	0.0000	4.70E0
x_9	0.9999	11.5	0.0002	4.32E0
R_A^2 = 0.9999, PRS_A = 1.78E-1				
C_T = 0.8727, C_T w/true = 0.9511				
SRD/RCC TEST				
x_2	NA	4.0	0.0000	NA
x_1	NA	4.0	0.0000	NA
R_A^2 = NA, PRS_A = NA				
C_T = 0.9317 C_T w/true = 1.0000				

Var	R^2	*df*	*p*-val	**PRS**
QUAD_REG				
x_2	0.5282	2.0	0.0000	9.75E2
x_1	0.9295	3.0	0.0000	1.55E2
R_A^2 = 0.9283, PRS_A = 1.47E2				
C_T = 0.9235, C_T w/true = 1.0000				
RP_REG				
x_2	0.5597	16.0	0.0000	1.26E3
x_1	0.9987	56.0	0.0000	1.28E1
x_{10}	0.9991	29.0	0.0000	1.24E1
R_A^2 = 0.9986, PRS_A = 4.33E0				
C_T = 0.9712, C_T w/true = 0.9712				
TRUE MODEL				
x_2	0.5196	NA	NA	NA
x_1	1.0000	NA	NA	NA
R_A^2 = NA, PRS_A = NA				
C_T = NA, C_T w/true = 1.0000				

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[a] Table structure same as described in footnotes to Table 1.

Table 3. Sensitivity Analyses for Analytic Test Model $y_3 = f_3(x_1, x_2, \ldots, x_8)$[a]

Var	R^2	*df*	*p*-val	PRS
LIN_REG				
None	0.0000	0.0	NA	1.18E2
R_A^2 = 0.0000, PRS_A = 1.18E2				
C_T = 0.3333, C_T w/true = 0.5000				
LOESS				
x_1	0.7047	5.8	0.0000	3.68E1
x_2	0.9503	44.2	0.0000	9.64E0
x_3	0.9819	72.2	0.0000	1.96E1
R_A^2 = 0.9694, PRS_A = 6.11E0				
C_T = 1.0000, C_T w/true = 0.9726				
GAM				
x_1	0.7164	10.0	0.0000	3.64E1
x_2	0.9089	15.0	0.0000	1.37E1
x_3	0.9324	4.0	0.0000	1.05E1
x_4	0.9414	4.0	0.0000	9.45E0
R_A^2 = 0.9341, PRS_A = 8.76E0				
C_T = 0.9730, C_T w/true = 0.9863				

Var	R^2	*df*	*p*-val	PRS
RANK_REG				
None	0.0000	0.0	NA	2.27E6
R_A^2 = 0.0000, PRS_A = 2.27E6				
C_T = 0.3333, C_T w/true = 0.500				
PP_REG				
x_1	0.7177	9.9	0.0000	3.69E1
x_2	0.9123	13.6	0.0000	1.79E1
x_5	0.9329	12.7	0.0000	1.43E1
x_7	0.9493	13.8	0.0000	1.54E1
R_A^2 = 0.9392, PRS_A = 8.71E0				
C_T = 0.8541, C_T w/true = 0.9146				
SRD/RCC TEST				
x_1	NA	4.0	0.0000	NA
x_2	NA	4.0	0.0003	NA
R_A^2 = NA, PRS_A = NA				
C_T = 0.9373, C_T w/true = 0.9453				

Var	R^2	*df*	*p*-val	PRS
QUAD_REG				
x_1	0.6540	2.0	0.0000	4.19E1
x_2	0.8459	3.0	0.0000	1.92E1
x_3	0.8733	4.0	0.0000	1.63E1
x_4	0.8803	5.0	0.0063	1.61E1
x_6	0.8870	6.0	0.0123	1.60E1
R_A^2 = 0.8789, PRS_A = 1.53E1				
C_T = 0.9730, C_T w/true = 0.9866				
RP_REG				
x_1	0.7201	10.0	0.0000	4.06E1
x_2	0.9719	62.0	0.0000	8.17E0
x_3	0.9818	36.0	0.0000	9.23E0
R_A^2 = 0.9715, PRS_A = 5.99E0				
C_T = 0.9726, C_T w/true = 0.9726				
TRUE MODEL				
x_1	0.7115	NA	NA	NA
x_2	0.9546	NA	NA	NA
x_3	0.9891	NA	NA	NA
x_4	0.9996	NA	NA	NA
x_5	0.9997	NA	NA	NA
x_6	0.9998	NA	NA	NA
x_7	0.9999	NA	NA	NA
x_8	1.0000	NA	NA	NA
R_A^2 = NA, PRS_A = NA				
C_T = NA, C_T w/true = 1.0000				

[a] Table structure same as described in footnotes to Table 1.

Table 4. Sensitivity Analyses for Analytic Test Model $y_4 = f_4(x_1, x_2, x_3)$[a]

Var	$\boldsymbol{R^2}$	***df***	***p*-val**	**PRS**	**Var**	$\boldsymbol{R^2}$	***df***	***p*-val**	**PRS**	**Var**	$\boldsymbol{R^2}$	***df***	***p*-val**	**PRS**
LIN_REG					**RANK_REG**					**QUAD_REG**				
x_1	0.1756	1.0	0.0000	3.26E3	x_1	0.1599	1.0	0.0000	1.92E6	x_1	0.1768	2.0	0.0000	3.28E3
R_A^2 = 0.1728, PRS_A = 3.26E3					R_A^2 = 0.1571, PRS_A = 1.92E6					R_A^2 = 0.1713, PRS_A = 3.28E3				
C_T = 1.0000, C_T w/true = 0.6949					C_T = 0.9373, C_T w/true = 0.6949					C_T = 0.9373, C_T w/true = 0.6949				
LOESS					**PP_REG**					**RP_REG**				
x_2	0.5030	18.1	0.0000	2.21E3	x_2	0.4669	7.9	0.0000	2.21E3	x_2	0.5114	19.0	0.0000	2.53E3
x_1	0.7982	31.9	0.0000	1.13E3	x_3	0.5483	21.0	0.0012	2.68E3	x_1	0.8180	48.0	0.0000	1.57E3
x_3	0.9519	72.2	0.0000	1.39E3	R_A^2 = 0.4999, PRS_A = 2.19E3					x_3	0.9033	41.0	0.0000	1.79E3
R_A^2 = 0.9187, PRS_A = 5.40E2					C_T = 0.7675, C_T w/true = 0.9171					R_A^2 = 0.8486, PRS_A = 1.00E3				
C_T = 1.0000, C_T w/true = 1.0000					**SRD/RCC TEST**					C_T = 1.0000, C_T w/true = 1.0000				
GAM					x_1	NA	4.0	0.0000	NA	**TRUE MODEL**				
x_2	0.4736	10.0	0.0000	2.21E3	x_2	NA	4.0	0.0000	NA	x_2	0.4463	NA	NA	NA
x_1	0.7753	7.0	0.0000	9.81E2	x_6	NA	4.0	0.0017	NA	x_1	0.7593	NA	NA	NA
x_4	0.7920	10.0	0.0188	9.72E2	R_A^2 = NA, R_A^2 = NA					x_3	1.0000	NA	NA	NA
R_A^2 = 0.7714, PRS_A = 9.87E2					C_T = 0.9207 C_T w/true = 0.8586					R_A^2 = NA, PRS_A = NA				
C_T = 0.9744, C_T w/true = 0.9360										C_T = NA, C_T w/true = 1.0000				

[a] Table structure same as described in footnotes to Table 1.

Table 5. Independent (i.e., sampled) Variables Considered in Example Sensitivity Analyses for Two-Phase Fluid Flow (Source: Table 1, Ref. 7, and Table 1, Ref. 22)

ANHBCEXP—Brooks-Corey pore distribution parameter for anhydrite (dimensionless). Distribution: Student's with 5 degrees of freedom. Range: 0.491 to 0.842. Mean, Median: 0.644, 0.644.

ANHBCVGP—Pointer variable for selection of relative permeability model for use in anhydrite. Distribution: Discrete with 60% 0, 40% 1. Value of 0 implies Brooks-Corey model; value of 1 implies van Genuchten-Parker model.

ANHCOMP—Bulk compressibility of anhydrite (Pa^{-1}). Distribution: Student's with 3 degrees of freedom. Range: 1.09×10^{-11} to 2.75×10^{-10} Pa^{-1}. Mean, Median: 8.26×10^{-11} Pa^{-1}, 8.26×10^{-11} Pa^{-1}. Correlation: –0.99 rank correlation[23, 24] with *ANHPRM*.

ANHPRM—Logarithm of anhydrite permeability (m^2). Distribution: Student's with 5 degrees of freedom. Range: –21.0 to –17.1 (i.e., permeability range is 1×10^{-21} to $1 \times 10^{-17.1}$ m^2). Mean, Median: –18.9, –18.9. Correlation : –0.99 rank correlation with *ANHCOMP*.

ANRBRSAT—Residual brine saturation in anhydrite (dimensionless). Distribution: Student's with 5 degrees of freedom. Range: 7.85×10^{-3} to 1.74×10^{-1}. Mean, Median: 8.36×10^{-2}, 8.36×10^{-2}.

ANRGSSAT—Residual gas saturation in anhydrite (dimensionless). Distribution: Student's with 5 degrees of freedom. Range: 1.39×10^{-2} to 1.79×10^{-1}. Mean, median: 7.71×10^{-2}, 7.71×10^{-2}.

BHPRM—Logarithm of borehole permeability (m^2). Distribution: Uniform. Range: –14 to –11 (i.e., permeability range is 1×10^{-14} to 1×10^{-11} m^2). Mean, median: –12.5, –12.5.

BPCOMP—Logarithm of bulk compressibility of brine pocket (Pa^{-1}). Distribution: Triangular. Range: –11.3 to –8.00 (i.e., bulk compressibility range is $1 \times 10^{-11.3}$ to 1×10^{-8} Pa^{-1}). Mean, mode: –9.80, –10.0. Correlation: –0.75 rank correlation with *BPPRM*.

BPINTPRS— Initial pressure in brine pocket (Pa). Distribution: Triangular. Range: 1.11×10^{7} to 1.70×10^{7} Pa. Mean, mode: 1.36×10^{7} Pa, 1.27×10^{7} Pa.

BPPRM— Logarithm of intrinsic brine pocket permeability (m^2). Distribution: Triangular. Range: –14.7 to –9.80 (i.e., permeability range is $1 \times 10^{-14.7}$ to $1 \times 10^{-9.80}$ m^2). Mean, mode: –12.1, –11.8. Correlation: –0.75 rank correlation with *BPCOMP*.

BPVOL— Pointer variable for selection of brine pocket volume. Distribution: Discrete, with integer values 1, 2, ..., 32 equally likely.

HALCOMP—Bulk compressibility of halite (Pa^{-1}). Distribution: Uniform. Range: 2.94×10^{-12} to 1.92×10^{-10} PA^{-1}. Mean, median: 9.75×10^{-11} Pa^{-1}, 9.75×10^{-11} Pa^{-1}. Correlation: –0.99 rank correlation with *HALPRM*.

HALPOR—Halite porosity (dimensionless). Distribution: Piecewise uniform. Range: 1.0×10^{-3} to 3×10^{-2}. Mean, median: 1.28×10^{-2}, 1.00×10^{-2}.

HALPRM—Logarithm of halite permeability (m^2). Distribution: Uniform. Range: –24 to –21 (i.e., permeability range is 1×10^{-24} to 1×10^{-21} m^2). Mean, median: –22.5, –22.5. Correlation: –0.99 rank correlation with *HALCOMP*.

Table 5. Independent (i.e., sampled) Variables Considered in Example Sensitivity Analyses for Two-Phase Fluid Flow (Source: Table 1, Ref. 7, and Table 1, Ref. 22) (Continued)

SALPRES—Initial brine pressure, without the repository being present, at a reference point located in the center of the combined shafts at the elevation of the midpoint of Marker Bed (MB) 139 (Pa). Distribution: Uniform. Range: 1.104×10^7 to 1.389×10^7 Pa. Mean, median: 1.247×10^7 Pa, 1.247×10^7 Pa.

SHBCEXP—Brooks-Corey pore distribution parameter for shaft (dimensionless). Distribution: Piecewise uniform. Range: 0.11 to 8.10. Mean, median: 2.52, 0.94.

SHPRMASP—Logarithm of permeability (m^2) of asphalt component of shaft seal (m^2). Distribution: Triangular. Range: –21 to –18 (i.e., permeability range is 1×10^{-21} to 1×10^{-18} m^2). Mean, mode: –19.7, –20.0.

SHPRMCLY—Logarithm of permeability (m^2) for clay components of shaft. Distribution: Triangular. Range: –21 to –17.3 (i.e., permeability range is 1×10^{-21} to $1 \times 10^{-17.3}$ m^2). Mean, mode: –18.9, –18.3.

SHPRMCON—Same as *SHPRMASP* but for concrete component of shaft seal for 0 to 400 yr. Distribution: Triangular. Range: –17.0 to –14.0 (i.e., permeability range is 1×10^{-17} to 1×10^{-14} m^2). Mean, mode: –15.3, –15.0.

SHPRMDRZ—Logarithm of permeability (m^2) of DRZ surrounding shaft. Distribution: Triangular. Range: –17.0 to –14.0 (i.e., permeability range is 1×10^{-17} to 1×10^{-14} m^2). Mean, mode: –15.3, –15.0.

SHPRMHAL—Pointer variable (dimensionless) used to select permeability in crushed salt component of shaft seal at different times. Distribution: Uniform. Range: 0 to 1. Mean, mode: 0.5, 0.5. A distribution of permeability (m^2) in the crushed salt component of the shaft seal is defined for each of the following time intervals: [0, 10 yr], [10, 25 yr], [25, 50 yr], [50, 100 yr], [100, 200 yr], [200, 10000 yr]. *SHPRMHAL* is used to select a permeability value from the cumulative distribution function for permeability for each of the preceding time intervals with result that a rank correlation of 1 exists between the permeabilities used for the individual time intervals.

SHRBRSAT—Residual brine saturation in shaft (dimensionless). Distribution: Uniform. Range: 0 to 0.4. Mean, median: 0.2, 0.2.

SHRGSSAT—Residual gas saturation in shaft (dimensionless). Distribution: Uniform. Range: 0 to 0.4. Mean, median: 0.2, 0.2.

WASTWICK—Increase in brine saturation of waste due to capillary forces (dimensionless). Distribution: Uniform. Range: 0 to 1. Mean, median: 0.5, 0.5.

WFBETCEL—Scale factor used in definition of stoichiometric coefficient for microbial gas generation (dimensionless). Distribution: Uniform. Range: 0 to 1. Mean, median: 0.5, 0.5.

WGRCOR—Corrosion rate for steel under inundated conditions in the absence of CO_2 (m/s). Distribution: Uniform. Range: 0 to 1.58×10^{-14} m/s. Mean, median: 7.94×10^{-15} m/s, 7.94×10^{-15} m/s.

WGRMICH—Microbial degradation rate for cellulose under humid conditions (mol/kg•s). Distribution: Uniform. Range: 0 to 1.27×10^{-9} mol/kg•s. Mean, median: 6.34×10^{-10} mol/kg•s, 6.34×10^{-10} mol/kg•s.

WGRMICI—Microbial degradation rate for cellulose under inundated conditions (mol/kg•s). Distribution: Uniform. Range: 3.17×10^{-10} to 9.51×10^{-9} mol/kg•s. Mean, median: 4.92×10^{-9} mol/kg•s, 4.92×10^{-9} mol/kg•s.

Table 5. Independent (i.e., sampled) Variables Considered in Example Sensitivity Analyses for Two-Phase Fluid Flow (Source: Table 1, Ref. 7, and Table 1, Ref. 22) (Continued)

WMICDFLG—Pointer variable for microbial degradation of cellulose. Distribution: Discrete, with 50% 0, 25% 1, 25% 2. *WMICDFLG* = 0, 1, 2 implies no microbial degradation of cellulose, microbial degradation of only cellulose, microbial degradation of cellulose, plastic, and rubber.

WRBRNSAT—Residual brine saturation in waste (dimensionless). Distribution: Uniform. Range: 0 to 0.552. Mean, median: 0.276, 0.276.

WRGSSAT—Residual gas saturation in waste (dimensionless). Distribution: Uniform. Range: 0 to 0.15. Mean, median: 0.075, 0.075.

Table 6. Time-Dependent Two-Phase Fluid Flow Results for a Drilling Intrusion at 1000 yr that Penetrates the Repository and an Underlying Region of Pressurized Brine (i.e., an E1 intrusion at 1000 yr) Used to Illustrate Sensitivity Analysis Results

BRNREPTC: Cumulative brine flow (m^3) into repository (i.e., into region corresponding to Cells 596 – 625, 638 – 640 in Fig. 3, Ref. 12).

REP_SATB: Average brine saturation in waste panels not penetrated by the drilling intrusion (i.e., in the region corresponding to Cells 617 – 625 in Fig. 3, Ref. 12).

WAS_PRES: Pressure (Pa) in waste panel penetrated by the drilling intrusion (i.e., in the region corresponding to Cells 596 – 616 in Fig. 3, Ref. 12).

Note 1: Effects of the drilling intrusion are only manifested for times greater than 1000 yr. Conditions for times less than or equal to 1000 yr are the same as for undisturbed conditions (i.e., E0 conditions in the terminology of the 1996 WIPP CCA).

Note 2: Suffixes of *.1K* and *.10K* are appended to variable names to indicate results at 1000 and 10,000 years, respectively.

Table 7. Sensitivity Analyses for Cumulative Brine Flow at 1000 yr into Repository (*BRNREPTC.1K*) for Undisturbed Conditions[a]

Var	R^2	*df*	*p*-value	*PRS*
LIN_REG				
HALPOR	0.9607	1.0	0.0000	8.09E8
WMICDFLG	0.9704	1.0	0.0000	6.12E8
ANHPRM	0.9785	1.0	0.0000	4.57E8
HALPRM	0.9801	1.0	0.0000	4.26E8
WRBRNSAT	0.9813	1.0	0.0000	4.02E8
WASTWICK	0.9825	1.0	0.0000	3.80E8
SALPRES	0.9831	1.0	0.0019	3.70E8
WGRCOR	0.9836	1.0	0.0032	3.62E8
R^2_A = 0.9831, PRS_A = 3.55E8, C_T = 0.9221				
QUAD_REG				
HALPOR	0.9657	2.0	0.0000	7.09E8
ANHPRM	0.9813	3.0	0.0000	4.15E8
WMICDFLG	0.9897	4.0	0.0000	2.42E8
HALPRM	0.9916	5.0	0.0000	2.08E8
WGRCOR	0.9934	6.0	0.0000	1.75E8
WASTWICK	0.9944	7.0	0.0000	1.56E8
SALPRES	0.9955	8.0	0.0000	1.40E8
WRBRNSAT	0.9964	9.0	0.0000	1.17E8
SHPRMDRZ	0.9968	10.0	0.0046	1.14E8
WRGSSAT	0.9971	11.0	0.0041	1.07E8
SHPRMCLY	0.9975	12.0	0.0025	1.04E8
R^2_A = 0.9966, PRS_A = 9.32E7, C_T = 0.9211				
PP_REG				
HALPOR	0.9659	2.9	0.0000	7.10E8
ANHPRM	0.9868	12.4	0.0000	3.47E8
WMICDFLG	0.9933	1.9	0.0000	1.97E8
SHPRMCON	0.9962	46.4	0.0000	3.07E8
HALPRM	0.9962	-42.1	0.0000	1.84E8
SALPRES	0.9984	51.3	0.0000	1.97E8
SHPRMASP	0.9989	32.0	0.0000	2.58E8
BPVOL	0.9992	3.3	0.0000	1.79E8
WRBRNSAT	0.9997	35.0	0.0000	2.68E8
R^2_A = 0.9995, PRS_A = 1.92E7, C_T = 0.8103				
SRD/RCC TEST				
HALPOR	NA	4.0	0.0000	NA
R^2_A = NA, PRS_A = NA, C_T = 1.0000				

Var	R^2	*df*	*p*-value	*PRS*
RANK_REG				
HALPOR	0.9550	1.0	0.0000	1.03E5
WMICDFLG	0.9658	1.0	0.0000	7.85E4
ANHPRM	0.9726	1.0	0.0000	6.37E4
HALPRM	0.9749	1.0	0.0000	5.87E4
WRBRNSAT	0.9764	1.0	0.0000	5.57E4
WASTWICK	0.9778	1.0	0.0000	5.29E4
SALPRES	0.9791	1.0	0.0000	5.00E4
WGRCOR	0.9800	1.0	0.0003	4.82E4
R^2_A = 0.9795, PRS_A = 4.78E4, C_T = 0.9224				
LOESS				
HALPOR	0.9657	2.3	0.0000	7.12E8
ANHPRM	0.9878	36.0	0.0000	3.75E8
WMICDFLG	0.9945	27.7	0.0000	2.49E8
WASTWICK	0.9963	24.6	0.0000	1.57E8
HALPRM	0.9979	44.2	0.0000	2.48E8
R^2_A = 0.9961, PRS_A = 1.45E8, C_T = 0.9203				
RP_REG				
HALPOR	0.9684	7.0	0.0000	7.26E8
ANHPRM	0.9870	15.0	0.0000	4.47E8
WMICDFLG	0.9924	2.0	0.0000	3.12E8
BPCOMP	0.9954	34.0	0.0000	3.80E8
ANRGSSAT	0.9960	13.0	0.0060	5.61E8
SALPRES	0.9965	0.0	0.0000	6.51E8
WASTWICK	0.9965	-19.0	0.0000	2.71E8
HALPRM	0.9974	7.0	0.0000	1.58E8
WGRCOR	0.9980	7.0	0.0000	9.18E7
SHBCEXP	0.9984	28.0	0.0119	1.54E8
SHPRMCON	0.9985	8.0	0.0085	7.69E7
R^2_A = 0.9978, PRS_A = 6.92E7, C_T = 0.9223				
GAM				
HALPOR	0.9661	4.0	0.0000	7.10E8
ANHPRM	0.9875	15.0	0.0000	3.10E8
WMICDFLG	0.9932	2.0	0.0000	1.75E8
HALPRM	0.9944	1.0	0.0000	1.47E8
WASTWICK	0.9951	2.0	0.0000	1.31E8
SALPRES	0.9956	2.0	0.0000	1.21E8
WGRCOR	0.9961	1.0	0.0000	1.10E8
WRBRNSAT	0.9964	1.0	0.0000	1.02E8
R^2_A = 0.9961, PRS_A = 8.90E7, C_T = 0.9593				

[a] Table structure same as described in footnotes to Table 1.

Table 8. Sensitivity Analyses for Cumulative Brine Flow at 10,000 yr into Repository (*BRNREPTC.10K*) for an E1 Intrusion at 1000 yr[a]

Var	R^2	*df*	*p*-value	*PRS*
LIN_REG				
BHPRM	0.2868	1.0	0.0000	1.64E11
BPCOMP	0.4590	1.0	0.0000	1.26E11
HALPOR	0.5645	1.0	0.0000	1.02E11
WMICDFLG	0.6267	1.0	0.0000	8.83E10
ANHPRM	0.6556	1.0	0.0000	8.24E10
BPVOL	0.6797	1.0	0.0000	7.73E10
SHRGSSAT	0.6886	1.0	0.0041	7.57E10
BPINTPRS	0.6976	1.0	0.0035	7.41E10
WGRCOR	0.7045	1.0	0.0098	7.30E10
WASTWICK	0.7109	1.0	0.0118	7.20E10
R_A^2 = 0.7009, PRS_A = 7.10E10, C_T = 0.9467				
QUAD_REG				
BHPRM	0.2923	2.0	0.0000	1.64E11
BPCOMP	0.4890	3.0	0.0000	1.23E11
WMICDFLG	0.6088	4.0	0.0000	9.62E10
HALPOR	0.7182	5.0	0.0000	7.18E10
ANHPRM	0.7831	6.0	0.0000	6.03E10
BPVOL	0.8215	7.0	0.0000	5.30E10
WGRCOR	0.8477	8.0	0.0000	4.89E10
BPINTPRS	0.8709	9.0	0.0000	4.67E10
SHPRMDRZ	0.8866	10.0	0.0004	4.44E10
SHPRMCON	0.8978	11.0	0.0093	4.43E10
SHPRMCLY	0.9087	12.0	0.0129	4.36E10
R_A^2 = 0.8770, PRS_A = 3.80E10, C_T = 0.9174				
PP_REG				
BHPRM	0.2916	1.7	0.0000	1.65E11
BPCOMP	0.4768	1.3	0.0000	1.29E11
HALPOR	0.6822	25.0	0.0000	1.09E11
WMICDFLG	0.8256	19.0	0.0000	7.06E10
ANRGSSAT	0.8389	2.6	0.0001	7.80E10
R_A^2 = 0.8069 PRS_A = 5.35E10, C_T = 0.3972				
SRD/RCC TEST				
BHPRM	NA	4.0	0.0000	NA
BPCOMP	NA	4.0	0.0000	NA
HALPOR	NA	4.0	0.0000	NA
BPPRM	NA	4.0	0.0000	NA
WMICDFLG	NA	4.0	0.0000	NA
BPVOL	NA	4.0	0.0057	NA
R_A^2 = NA, PRS_A = NA, C_T = 0.9225				

Var	R^2	*df*	*p*-value	*PRS*
RANK_REG				
BHPRM	0.3415	1.0	0.0000	1.50E6
BPCOMP	0.4874	1.0	0.0000	1.18E6
HALPOR	0.6065	1.0	0.0000	9.12E5
WMICDFLG	0.6778	1.0	0.0000	7.52E5
BPVOL	0.6974	1.0	0.0000	7.12E5
ANHPRM	0.7104	1.0	0.0003	6.87E5
BPINTPRS	0.7117	1.0	0.0063	6.75E5
R_A^2 = 0.7109, PRS_A = 6.70E5, C_T = 0.9629				
LOESS				
BHPRM	0.2933	2.3	0.0000	1.64E11
BPCOMP	0.5242	10.8	0.0000	1.22E11
HALPOR	0.7473	50.6	0.0000	1.03E11
ANHPRM	0.7404	-21.7	0.0012	8.87E10
WMICDFLG	0.8379	15.5	0.0000	6.17E10
BPVOL	0.8814	22.5	0.0000	5.83E10
R_A^2 = 0.8382, PRS_A = 5.07E10, C_T = 0.7243				
RP_REG				
BHPRM	0.2868	1.0	0.0000	1.66E11
BPCOMP	0.5244	11.0	0.0000	1.25E11
WMICDFLG	0.6582	12.0	0.0000	1.01E11
HALPOR	0.7899	16.0	0.0000	7.37E10
ANHPRM	0.8909	42.0	0.0000	5.95E10
HALPRM	0.9281	41.0	0.0002	9.02E10
BPPRM	0.9461	19.0	0.0003	7.32E10
R_A^2 = 0.8973, PRS_A = 4.49E10, C_T = 0.7110				
GAM				
BHPRM	0.2928	2.0	0.0000	1.64E11
BPCOMP	0.4880	2.0	0.0000	1.22E11
HALPOR	0.6011	4.0	0.0000	9.74E10
ANHPRM	0.6876	7.0	0.0000	8.03E10
WMICDFLG	0.7450	2.0	0.0000	6.60E10
BPVOL	0.7596	1.0	0.0000	6.28E10
SHRBRSAT	0.7846	10.0	0.0008	6.02E10
SHRGSSAT	0.7951	4.0	0.0099	5.90E10
WGRCOR	0.8042	2.0	0.0024	5.71E10
WASTWICK	0.8107	1.0	0.0028	5.58E10
SHPRMCLY	0.8181	2.0	0.0057	5.44E10
R_A^2 = 0.7924, PRS_A = 5.44E10, C_T = 0.8729				

[a] Table structure same as described in footnotes to Table 1.

Table 9. Sensitivity Analyses for Average Brine Saturation at 1000 yr in Waste Panels Not Penetrated by a Drilling Intrusion (*REP_SATB.1K*) for Undisturbed Conditions[a]

Var	R^2	*df*	*p*-value	*PRS*
LIN_REG				
HALPOR	0.5739	1.0	0.0000	1.30E2
WGRCOR	0.7398	1.0	0.0000	7.99E1
WMICDFLG	0.8267	1.0	0.0000	5.36E1
WASTWICK	0.8792	1.0	0.0000	3.77E1
SHRGSSAT	0.8819	1.0	0.0092	3.71E1
R_A^2 = 0.8799, PRS_A = 3.68E1, C_T = 0.9834				
QUAD_REG				
HALPOR	0.5835	2.0	0.0000	1.28E2
WGRCOR	0.7904	3.0	0.0000	6.59E1
WMICDFLG	0.9211	4.0	0.0000	2.53E1
WASTWICK	0.9804	5.0	0.0000	6.74E0
WRBRNSAT	0.9825	6.0	0.0000	6.35E0
SALPRES	0.9841	7.0	0.0002	6.04E0
ANHPRM	0.9853	8.0	0.0124	6.04E0
SHPRMDRZ	0.9864	9.0	0.0114	5.88E0
R_A^2 = 0.9841, PRS_A = 5.62E0, C_T = 0.9243				
PP_REG				
HALPOR	0.5822	2.0	0.0000	1.29E2
WGRCOR	0.8001	4.0	0.0000	6.44E1
WMICDFLG	0.9430	25.4	0.0000	2.31E1
WASTWICK	0.9926	12.7	0.0000	4.22E0
SHRGSSAT	0.9946	25.4	0.0000	5.43E0
BHPRM	0.9961	16.6	0.0000	5.74E0
R_A^2 = 0.9945 PRS_A = 2.36E0, C_T = 0.8598				
SRD/RCC TEST				
HALPOR	NA	4.0	0.0000	NA
WGRCOR	NA	4.0	0.0000	NA
WMICDFLG	NA	4.0	0.0000	NA
WASTWICK	NA	4.	0.0000	NA
R_A^2 = NA, PRS_A = NA, C_T = 0.9102				

Var	R^2	*df*	*p*-value	*PRS*
RANK_REG				
HALPOR	0.6141	1.0	0.0000	8.79E5
WGRCOR	0.7704	1.0	0.0000	5.27E5
WASTWICK	0.8516	1.0	0.0000	3.44E5
WMICDFLG	0.9201	1.0	0.0000	1.87E5
R_A^2 = 0.9190, PRS_A = 1.86E5, C_T = 0.9973				
LOESS				
HALPOR	0.5821	2.3	0.0000	1.28E2
WGRCOR	0.8025	9.7	0.0000	6.52E1
WMICDFLG	0.9593	67.3	0.0000	2.40E1
WASTWICK	0.9919	4.0	0.0000	5.10E0
R_A^2 = 0.9888, PRS_A = 4.69E0, C_T = 1.000				
RP_REG				
HALPOR	0.6461	10.0	0.0000	1.30E2
WGRCOR	0.8161	7.0	0.0000	7.84E1
WMICDFLG	0.9487	31.0	0.0000	2.82E1
WASTWICK	0.9896	42.0	0.0000	9.96E0
ANHBCVGP	0.9929	31.0	0.0000	1.09E1
R_A^2 = 0.9881, PRS_A = 6.01E0, C_T = 0.9664				
GAM				
HALPOR	0.5821	2.0	0.0000	1.28E2
WGRCOR	0.7564	2.0	0.0000	7.60E1
WMICDFLG	0.8409	2.0	0.0000	5.02E1
WASTWICK	0.8953	2.0	0.0000	3.36E1
R_A^2 = 0.8925, PRS_A = 3.33E1, C_T = 0.9546				

[a] Table structure same as described in footnotes to Table 1.

Table 10. Sensitivity Analyses for Average Brine Saturation at 10,000 yr in Waste Panels Not Penetrated by a Drilling Intrusion (*REP_SATB.10K*) for an E1 Intrusion at 1000 yr[a]

Var	R^2	*df*	*p*-value	*PRS*
LIN_REG				
WGRCOR	0.2803	1.0	0.0000	2.18E2
BHPRM	0.4359	1.0	0.0000	1.72E2
HALPOR	0.5111	1.0	0.0000	1.50E2
BPCOMP	0.5811	1.0	0.0000	1.30E2
SHRGSSAT	0.6048	1.0	0.0000	1.23E2
WASTWICK	0.6258	1.0	0.0001	1.18E2
WMICDFLG	0.6443	1.0	0.0001	1.12E2
ANHPRM	0.6601	1.0	0.0003	1.08E2
BPVOL	0.6696	1.0	0.0041	1.06E2
R^2_A = 0.6594, PRS_A = 1.06E2, C_T = 0.9003				
QUAD_REG				
WGRCOR	0.4232	2.0	0.0000	1.76E2
BHPRM	0.5992	3.0	0.0000	1.24E2
HALPOR	0.6717	4.0	0.0000	1.04E2
BPCOMP	0.7449	5.0	0.0000	8.48E1
WMICDFLG	0.7835	6.0	0.0000	7.48E1
WASTWICK	0.8101	7.0	0.0000	7.04E1
ANHPRM	0.8329	8.0	0.0000	6.66E1
SHRGSSAT	0.8496	9.0	0.0012	6.40E1
R^2_A = 0.8237, PRS_A = 6.22E1, C_T = 0.9120				
PP_REG				
WGRCOR	0.4736	4.3	0.0000	1.64E2
BHPRM	0.6472	5.5	0.0000	1.14E2
SHPRMCLY	0.7382	27.4	0.0000	1.14E2
BPCOMP	0.7954	-2.5	0.0000	9.98E1
HALPRM	0.8657	30.0	0.0000	9.16E1
BPVOL	0.8985	12.6	0.0000	1.06E2
R^2_A = 0.8632 PRS_A = 5.60E1, C_T = 0.6226				
SRD/RCC TEST				
WGRCOR	NA	4.0	0.0000	NA
BHPRM	NA	4.0	0.0000	NA
HALPOR	NA	4.0	0.0000	NA
BPCOMP	NA	4.0	0.0001	NA
BPPRM	NA	4.0	0.0144	NA
R^2_A = NA, PRS_A = NA, C_T = 0.9292				

Var	R^2	*df*	*p*-value	*PRS*
RANK_REG				
BHPRM	0.2619	1.0	0.0000	1.68E6
WGRCOR	0.4790	1.0	0.0000	1.19E6
HALPOR	0.5584	1.0	0.0000	1.02E6
BPCOMP	0.6226	1.0	0.0000	8.78E5
WASTWICK	0.6488	1.0	0.0000	8.23E5
WMICDFLG	0.6703	1.0	0.0000	7.78E5
SHRGSSAT	0.6815	1.0	0.0015	7.56E5
ANHPRM	0.6928	1.0	0.0012	7.35E5
BPVOL	0.7023	1.0	0.0026	7.17E5
R^2_A = 0.6931 PRS_A = 7.17E5, C_T = 0.8966				
LOESS				
WGRCOR	0.4751	5.6	0.0000	1.64E2
BHPRM	0.7118	29.1	0.0000	1.07E2
BPCOMP	0.7401	-11.3	0.0000	9.21E1
HALPOR	0.7968	14.1	0.0000	8.10E1
R^2_A = 0.7676, PRS_A = 8.00E1, C_T = 0.9203				
RP_REG				
WGRCOR	0.4836	7.0	0.0000	1.68E2
BHPRM	0.6905	10.0	0.0000	1.20E2
HALPOR	0.7689	14.0	0.0000	1.06E2
BPCOMP	0.8336	9.0	0.0000	7.66E1
WASTWICK	0.8740	20.0	0.0000	8.39E1
SHRGSSAT	0.8971	24.0	0.0047	7.77E1
R^2_A = 0.8570, PRS_A = 5.99E1, C_T = 0.8300				
GAM				
WGRCOR	0.4719	4.0	0.0000	1.63E2
BHPRM	0.6523	2.0	0.0000	1.09E2
HALPOR	0.7227	4.0	0.0000	8.88E1
BPCOMP	0.7732	1.0	0.0000	7.35E1
WASTWICK	0.7994	4.0	0.0000	6.71E1
ANHPRM	0.8169	2.0	0.0000	6.24E1
WMICDFLG	0.8443	2.0	0.0000	5.35E1
R^2_A = 0.8338, PRS_A = 5.34E1, C_T = 0.9000				

[a] Table structure same as described in footnotes to Table 1.

Table 11. Sensitivity Analysis for Pressure at 1000 yr in Waste Panel Penetrated by a Drilling Intrusion (*WAS_PRES.1K*) for Undisturbed Conditions[a]

Var	R^2	*df*	*p*-value	*PRS*
LIN_REG				
WMICDFLG	0.8457	1.0	0.0000	4.67E1
WGRCOR	0.9193	1.0	0.0000	2.46E1
WASTWICK	0.9503	1.0	0.0000	1.53E1
HALPOR	0.9535	1.0	0.0000	1.44E1
ANHPRM	0.9559	1.0	0.0001	1.38E1
WGRMICI	0.9573	1.0	0.0016	1.34E1
ANHBCVGP	0.9582	1.0	0.0161	1.32E1
R_A^2 = 0.9572, PRS_A = 1.32E1, C_T = 0.9401				
QUAD_REG				
WMICDFLG	0.8564	2.0	0.0000	4.37E1
WGRCOR	0.9451	3.0	0.0000	1.71E1
WASTWICK	0.9769	4.0	0.0000	7.44E0
HALPOR	0.9861	5.0	0.0000	4.64E0
WGRMICI	0.9886	6.0	0.0000	4.10E0
ANHPRM	0.9900	7.0	0.0000	3.74E0
WGRMICH	0.9908	8.0	0.0067	3.70E0
R_A^2 = 0.9895, PRS_A = 3.57E0, C_T = 0.9569				
PP_REG				
WMICDFLG	0.8564	2.0	0.0000	4.37E1
WGRCOR	0.9458	4.3	0.0000	1.71E1
WASTWICK	0.9718	3.8	0.0000	8.29E0
WRBRNSAT	0.9827	30.5	0.0000	9.15E0
HALPOR	0.9904	9.9	0.0000	5.49E0
SHBCEXP	0.9947	27.8	0.0000	6.68E0
HALPRM	0.9960	19.7	0.0000	6.16E0
ANHBCVGP	0.9963	1.5	0.0002	6.72E0
SHRBRSAT	0.9978	21.3	0.0000	8.47E0
R_A^2 = 0.9963 PRS_A = 1.87E0, C_T = 0.8671				
SRD/RCC TEST				
WMICDFLG	NA	4.0	0.0000	NA
WGRCOR	NA	4.0	0.0000	NA
WASTWICK	NA	4.0	0.0001	NA
SHPRMASP	NA	4.0	0.0120	NA
R_A^2 = NA, PRS_A = NA, C_T = 0.8697				

Var	R^2	*df*	*p*-value	*PRS*
RANK_REG				
WMICDFLG	0.7830	1.0	0.0000	4.94E5
WGRCOR	0.8909	1.0	0.0000	2.51E5
WASTWICK	0.9366	1.0	0.0000	1.47E5
HALPOR	0.9427	1.0	0.0000	1.34E5
ANHPRM	0.9456	1.0	0.0001	1.28E5
WGRMICI	0.9468	1.0	0.0094	1.26E5
R_A^2 = 0.9457, PRS_A = 1.26E5, C_T = 0.9834				
LOESS				
WMICDFLG	0.8564	2.0	0.0000	4.37E1
WGRCOR	0.9528	25.4	0.0000	1.74E1
WASTWICK	0.9852	47.0	0.0000	8.04E0
HALPOR	0.9924	9.0	0.0000	5.25E0
WGRMICI	0.9949	44.3	0.0018	9.02E0
R_A^2 = 0.9911, PRS_A = 4.68E0, C_T = 0.9755				
RP_REG				
WMICDFLG	0.8564	4.0	0.0000	4.45E1
WGRCOR	0.9505	13.0	0.0000	1.78E1
WASTWICK	0.9782	13.0	0.0000	9.54E0
HALPOR	0.9929	52.0	0.0000	6.55E0
SHPRMCON	0.9940	19.0	0.0157	8.38E0
WGRMICI	0.9955	19.0	0.0001	1.03E1
R_A^2 = 0.9924, PRS_A = 3.80E0, C_T = 0.9593				
GAM				
WMICDFLG	0.8457	1.0	0.0000	4.67E1
WGRCOR	0.9338	3.0	0.0000	2.05E1
WASTWICK	0.9654	2.0	0.0000	1.09E1
HALPOR	0.9695	1.0	0.0000	9.72E0
ANHPRM	0.9721	2.0	0.0000	8.99E0
WGRMICI	0.9732	2.0	0.0042	8.79E0
HALPRM	0.9763	15.0	0.0025	8.61E0
R_A^2 = 0.9741, PRS_A = 8.55E0, C_T = 0.8834				

[a] Table structure same as described in footnotes to Table 1.

Table 12. Sensitivity Analyses for Pressure at 10,000 yr in Waste Panel Penetrated by a Drilling Intrusion (*WAS_PRES.10K*) for an E1 Intrusion at 1000 yr[a]

Var	R^2	*df*	*p*-value	*PRS*
LIN_REG				
HALPRM	0.1188	1.0	0.0000	2.67E2
BPCOMP	0.1724	1.0	0.0000	2.53E2
ANHPRM	0.2168	1.0	0.0001	2.41E2
HALPOR	0.2428	1.0	0.0016	2.35E2
BPVOL	0.2679	1.0	0.0017	2.28E2
R_A^2 = 0.2554, PRS_A = 2.28E2, C_T = 0.7730				
QUAD_REG				
BHPRM	0.4550	2.0	0.0000	1.66E2
HALPRM	0.5499	3.0	0.0000	1.39E2
BPCOMP	0.6201	4.0	0.0000	1.22E2
ANHPRM	0.6873	5.0	0.0000	1.05E2
HALPOR	0.7299	6.0	0.0000	9.52E1
WGRCOR	0.7713	7.0	0.0000	8.59E1
WMICDFLG	0.8030	8.0	0.0000	7.83E1
BPVOL	0.8273	9.0	0.0001	7.41E1
BPINTPRS	0.8456	10.0	0.0018	7.28E1
R_A^2 = 0.8116, PRS_A = 6.92E1, C_T = 0.8646				
PP_REG				
BHPRM	0.4992	9.7	0.0000	1.62E2
HALPRM	0.5882	4.7	0.0000	1.40E2
WGRCOR	0.6794	20.5	0.0000	1.45E2
BPCOMP	0.7181	-15.0	0.0000	1.13E2
HALPOR	0.8261	24.9	0.0000	1.14E2
R_A^2 = 0.7955, PRS_A = 7.30E1, C_T = 0.6399				
SRD/RCC TEST				
BHPRM	NA	4.0	0.0000	NA
HALPRM	NA	4.0	0.0000	NA
BPCOMP	NA	4.0	0.0002	NA
ANHPRM	NA	4.0	0.0011	NA
BPVOL	NA	4.0	0.0149	NA
R_A^2 = NA, PRS_A = NA, C_T = 0.9074				

Var	R^2	*df*	*p*-value	*PRS*
RANK_REG				
HALPRM	0.1207	1.0	0.0000	2.00E6
BPCOMP	0.1716	1.0	0.0000	1.90E6
ANHPRM	0.2023	1.0	0.0008	1.84E6
BPVOL	0.2258	1.0	0.0030	1.80E6
HALPOR	0.2494	1.0	0.0026	1.76E6
SHRGSSAT	0.2636	1.0	0.0182	1.74E6
R_A^2 = 0.2485, PRS_A = 1.74E6, C_T = 0.8835				
LOESS				
BHPRM	0.5312	17.5	0.0000	1.59E2
HALPRM	0.6332	16.4	0.0000	1.39E2
ANHPRM	0.7444	32.4	0.0000	1.23E2
BPCOMP	0.8371	39.8	0.0000	1.35E2
R_A^2 = 0.7477, PRS_A = 1.18E2, C_T = 0.7733				
RP_REG				
BHPRM	0.5294	16.0	0.0000	1.69E2
WGRCOR	0.6588	26.0	0.0000	1.73E2
BPCOMP	0.7628	17.0	0.0000	1.45E2
ANHPRM	0.8049	8.0	0.0000	1.21E2
HALPRM	0.8540	4.0	0.0000	1.70E2
WRBRNSAT	0.9230	52.0	0.0000	8.21E1
BPINTPRS	0.9495	34.0	0.0007	1.16E2
R_A^2 = 0.8937, PRS_A = 6.74E1, C_T = 0.8632				
GAM				
BHPRM	0.4992	10.0	0.0000	1.61E2
HALPRM	0.5613	1.0	0.0000	1.42E2
ANHPRM	0.6305	4.0	0.0000	1.23E2
BPCOMP	0.6884	2.0	0.0000	1.06E2
HALPOR	0.7296	4.0	0.0000	9.46E1
WGRCOR	0.7564	4.0	0.0000	8.78E1
BPVOL	0.7666	1.0	0.0007	8.47E1
SHRBRSAT	0.7776	4.0	0.0111	8.30E1
SHRGSSAT	0.7833	1.0	0.0084	8.16E1
BPINTPRS	0.7891	1.0	0.0075	7.99E1
R_A^2 = 0.7638, PRS_A = 7.96E1, C_T = 0.7460				

[a] Table structure same as described in footnotes to Table 1.