Sensitivity of the CRA-2014 Performance Assessment Releases to Parameters

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Introduction

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations (CFR), Part 191. The DOE demonstrates compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194 by means of performance assessment (PA) calculations performed by Sandia National Laboratories (SNL). WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The models used in PA are maintained and updated with new information as part of an ongoing process. Improved information regarding important WIPP features, events, and processes typically results in refinements and modifications to PA models and the parameters used in them. Planned changes to the repository and/or the components therein also result in updates to WIPP PA models. WIPP PA models are used to support the repository recertification process that occurs at five-year intervals following the receipt of the first waste shipment at the site in 1999.

PA calculations were included in the 1996 Compliance Certification Application (CCA) (U.S. DOE 1996), and in a subsequent Performance Assessment Verification Test (PAVT) (MacKinnon and Freeze 1997a, 1997b and 1997c). Based in part on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the regulatory containment criteria. The facility was approved for disposal of transuranic waste in May 1998 (U.S. EPA 1998). PA calculations were an integral part of the 2004 Compliance Recertification Application (CRA-2004) (U.S. DOE 2004). During their review of the CRA-2004, the EPA requested an additional PA calculation, referred to as the CRA-2004 Performance Assessment Baseline Calculation (PABC) (Leigh et al. 2005), be conducted with modified assumptions and parameter values (Cotsworth 2005). Following review of the CRA-2004 and the CRA-2004 PABC, the EPA recertified the WIPP in March 2006 (U.S. EPA 2006).

PA calculations were completed for the second WIPP recertification and documented in the 2009 Compliance Recertification Application (CRA-2009). The CRA-2009 PA resulted from continued review of the CRA-2004 PABC, including a number of technical changes and corrections, as well as updates to parameters and improvements to the PA computer codes (Clayton et al. 2008). To incorporate additional information which was received after the CRA-2009 PA was completed, but before the submittal of the CRA-2009, the EPA requested an additional PA calculation, referred to as the 2009 Compliance Recertification Application Performance Assessment Baseline Calculation (PABC-2009) (Clayton et al. 2010), be undertaken which included updated information (Cotsworth 2009). Following the completion and submission of the PABC-2009, the WIPP was recertified in 2010 (U.S. EPA 2010).

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The Land Withdrawal Act (U.S. Congress 1992) requires that the DOE apply for WIPP recertification every five years following the initial 1999 waste shipment. The 2014 Compliance Recertification Application (CRA-2014) will be the third WIPP recertification application submitted by the DOE for EPA approval. The PA executed by SNL in support of the CRA-2014 is detailed in AP-164 (Camphouse 2013). The CRA-2014 PA includes a number of technical changes and parameter refinements, as well as a redesigned WIPP panel closure system. Results found in the CRA-2014 PA are compared to those obtained in the PABC-2009 in order to assess repository performance in terms of the current regulatory baseline. This report documents the analysis of the sensitivity of modeled releases to input parameters sampled using LHS for the CRA-2014 PA.

The STEPWISE Procedure

The code STEPWISE version 2.21 was used to determine the relative importance of the sampled parameters in the CRA-2014. STEPWISE receives sampled input parameter values and calculated release data that correspond to those input parameters. The release data are represented by the means across 10,000 futures for each vector. STEPWISE relates the sampled input parameter values to the vector means by performing a multiple regression analysis and reporting the results in tables.

WIPP PA employs stepwise linear multiple regression to evaluate the relative importance of the various sampled parameters on the estimates of potential releases. In the forward stepwise approach used by STEPWISE, a sequence of regression models is constructed, starting with the input parameter that has the strongest simple correlation with the output variable. Partial correlations between the output and the remaining variables are then computed. The partial correlations remove the linear effects of variables already included in the model. The variable having the largest significant partial correlation coefficient is added next, and the partial correlations for the remaining input variables are recomputed. Significance is determined using an F-test, and the significance level for adding an input variable to the model is $1-\alpha_{in}$, where α_{in} is the significance level for a Type I error that is set by the analyst. The F-test compares the variability contributed by the variable to the variability not accounted for by the regression, i.e. the variability of the residuals. By default STEPWISE sets $\alpha_{in} = 0.05$, so that one is 95% confident that there is a partial correlation between the input and output variables. This process is repeated until no remaining variables have significant correlations with the output variable. Variable excluded from the regression model contribute no significant information in relation to the unexplained variability and hence the results are judged to be relatively insensitive to those parameters. The method does not guarantee that the relative contributions of model parameters to the R^2 will always be smaller with increasing rank but this is often the case.

Input variables that are added to the regression model are not necessarily retained. For an input variable to be retained, its regression coefficient, i.e. the linear contribution of an input to the prediction of the output variable, must be statistically distinguishable from zero. A t-test is used to determine whether a regression coefficient is significantly different than zero. The t-test evaluates the null hypothesis that the regression coefficient is zero. The hypothesis

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is not rejected when random effects can give rise to the observed regression coefficient with probability α_{out} . The random effects are caused by the stochastic variability contributed by the input variables not in the regression model. In other words, the hypothesis is rejected, and the variable is included in the model when the $1-\alpha_{out}$ confidence interval of the regression coefficient does not encompass zero. By default the STEPWISE α_{out} -value for allowing a variable to enter the regression model is 0.05. Thus, in the default case, one is 95% confident that the input variables make a linear contribution to the response of the output variable. The user may specify different α -values in the input control file. However, the value allowing a variable to enter the model, α_{in} , must be less than or equal to the value by which a variable is allowed to leave the model, α_{out} , to avoid looping. In the following analyses, α_{in} was 0.05, and α_{out} was 0.05.

The predicted error sum of squares (PRESS) was computed to detect over-fitting of the regression model to the data. Over-fitting can occur when the regression methodology causes the fit to favor specific points rather than the general shape of the data curve. In such a case the minimum value of PRESS may occur earlier than the last step in the regression analysis. No such condition was observed in any of the rank correlation analyses reported herein.

This report documents the results of the CRA-2014 PA sensitivity analysis and shows, for comparison, the results obtained for the PABC-2009 analysis (Kirchner 2010). The details of run control for the PRECCDFGF and CCDFGF results presented herein are documented in Long (2013). The files of mean values of releases, STP_CRA14_MEANS_Rr.TRN, were generated from the CCGF_CRA14_Rr.OUT files using the Microsoft® Access 2010 database CCDFGF_Analysis.mdb. The CCDFGF output files store the mean values and those mean values are extracted from those files along with the "binned" data. The "bins" are a series of equally spaced intervals on a logarithmic scale that encompass the data. Each datum is assigned to a bin and the frequency of values within the bin tabulated. The databases are provided on the attached CD in zipped format and the CRA14_ANALYSISDATABASE.ZIP file is also stored in the CMS library LIBCRA14_STPW (Attachment 1).

The input files for STEPWISE use short names for input parameters rather than material:property designations used in other codes. These short names are required because of a limitation in the length of variable names in STEPWISE. Table 1 associates these names with the material and property names. In addition, three variables are created in STEPWISE through transformation of the variable GLOBAL:OXSTAT, the indicator variable for oxidation states of uranium and plutonium. GLOBAL:OXSTAT is sampled as a [0,1) uniform distribution but is treated in the code as a Bernoulli distribution (a distribution having only two discrete states). The computed variable OXSTAT is assigned 0 if GLOBAL:OXSTAT is less than 0.5 and is assigned 1 otherwise. The other two computed variables represent the K_ds for the +VI and +IV oxidation states of uranium and plutonium, respectively. A K_d value represents the matrix:water partitioning coefficient. If GLOBAL:OXSTAT is 0 then CMKDU is assigned U+6:MKD_U and CMKDPU is assigned PU+4:MKD_PU, i.e. the K_ds for the +VI and +IV oxidation states of uranium and plutonium,

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respectively. If GLOBAL:OXSTAT is 1 then CMKDU is assigned U+4:MKD_U and CMKDPU is assigned PU+3:MKD_PU, i.e. the K_ds for the +IV and +III oxidation states of uranium and plutonium, respectively. In the discussion below these variables are referenced as Composite:MKD_U and Composite:MKD_PU in order to denote their status as composites of pairs of sampled parameters.

Table 1. Material and property values associated with the variable names used in the CRA-2014 PA sensitivity analysis. References in this table refer to U. S. DOE (2004).

Material	Property	Variable Name	Description
Name AM+3	Name MKD_AM	СМКДАМЗ	Matrix distribution coefficient (m ³ /kg) for Am in +3 oxidation state. Defines K _{dk} in Equation (231).
BH_SAND	PRMX_LOG	BHPERM	Logarithm of intrinsic permeability (m ²) of the silty sand-filled borehole (Table PA-5). Used in regions Upper Borehole and Lower Borehole in Figure PA-8.
BOREHOLE	DOMEGA	DOMEGA	Drill string angular velocity (rad/s). Equation (112b).
BOREHOLE	TAUFAIL	WTAUFAIL	Shear strength of waste (Pa). Equation (111).
CASTILER	COMP_RCK	врсомр	Bulk compressibility (Pa–1) of Castile brine reservoir. Equation (29) for region CASTILER of Figure PA-8
CASTILER	PRESSURE	BPINTPRS	Initial brine pore pressure in the Castile brine reservoir. Equation (50) for region CASTILER in Figure PA-8.
CASTILER	PRMX_LOG	BPPRM	Logarithm of intrinsic permeability (m ²) of the Castile brine reservoir. Used in region CASTILER in Figure PA-8.
CONC_PLG	PRMX_LOG	PLGPRM	Logarithm of intrinsic permeability (m ²) of the concrete borehole plugs (Table PA-5). Used in region Borehole Plugs in Figure PA-8.
CULEBRA	APOROS	CFRACPOR	Culebra fracture (i.e., advective) porosity (dimensionless). Equation (223).
CULEBRA	DPOROS	CMTRXPOR	Culebra matrix (i.e., diffusive) porosity (dimensionless). Equation (230).

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Material Name	Property Name	Variable Name	Description
CULEBRA	HMBLKLT	CFRACSP (previously CUHMBLKLT)	Culebra fracture spacing (m). Equal to half the distance between fractures (i.e., the Culebra half matrix block length). Defines B in Equation (236) and Figure PA-26.
CULEBRA	MINP_FAC	CTRANSFM	Multiplier (dimensionless) applied to transmissivity of the Culebra within the land withdrawal boundary after mining of potash reserves. Defines MF in Equation (216) (see section PA-4.8.2).
DRZ_1	PRMX_LOG	DRZPRM	Logarithm of intrinsic permeability (m ²) of the DRZ. Used in regions Upper DRZ and Lower DRZ in Figure PA-8.
DRZ_PCS	PRMX_LOG	DRZPCPRM	Logarithm of intrinsic permeability (m ²) of the DRZ immediately above the panel closure concrete (Section PA-4.2.8.3). Used in region DRZ_PCS in Figure PA-8.
GLOBAL	CLIMTIDX	CCLIMSF	Climate scale factor (dimensionless) for Culebra flow field. Defines SFC in Equation (221).
GLOBAL	OXSTAT	WOXSTAT	Indicator variable for elemental oxidation states (dimensionless). WOXSTAT <= 0.05 indicates use of CMKDPU3, CMKDU4, WSOLPU3C, WSOLPUS, WSOLU4C, and WSOLU4S. WOXSTAT >0.05 implies use of CMKDPU4, CMKDU6, WSOLPU4C, WSOLPU4S, WSOLU6C, and WSOLU6S.
GLOBAL	PBRINE	PBRINE , (previously BPPROB)	Probability that a drilling intrusion penetrates pressurized brine in the Castile Formation. Defines pB1; see Section PA-3.5.
GLOBAL	TRANSIDX	CTRAN	Indicator variable for selecting transmissivity field. See Section PA-4.8.2.
PCS_T1	PORE_DIS	T1PDIS	Brooks-Corey pore distribution parameter
PCS_T1	POROSITY	T1POROS	Effective porosity

Material	Property	Variable Name	Description
Name PCS_T1	Name PRMX_LOG	T1PRMX	Log of intrinsic permeability, X-direction
PCS_T1	SAT_RBRN	T1SRBRN	Residual Brine Saturation
PCS_T1	SAT_RGAS	T1SRGAS	Residual Gas Saturation
PCS_T2	POR2PERM	T2P2PERM	Distribution used to calculate permeability from sampled porosity values
PCS_T2	POROSITY	T2POROS	Effective porosity
PCS_T3	POROSITY	T3POROS	Effective porosity
PHUMOX3	PHUMCIM	WPHUMOX3	Ratio (dimensionless) of concentration of actinides attached to humic colloids to dissolved concentration of actinides for oxidation state +III in Castile brine. Defines SFHum(Castile, +3, Am) and SFHum(Castile, +3, Pu) for Equation (90).
PU+3	MKD_PU	СМКДРИЗ	Matrix distribution coefficient (m ³ /kg) for Pu in +3 oxidation state. Defines Kdk in Equation (231).
PU+4	MKD_PU	CMKDPU4	Matrix distribution coefficient (m3/kg) for Pu in +4 oxidation state. Defines K _{dk} in Equation (231).
S_HALITE	COMP_RCK	HALCROCK	Bulk compressibility of halite (Pa–1). Equation (31) for region Salado of Figure PA-8.
S_HALITE	POROSITY	HALPOR	Halite porosity (dimensionless). Equation (25g) for region Salado in Figure PA-8.
S_HALITE	PRESSURE	SALPRES	Initial brine pore pressure (Pa) in the Salado halite, applied at an elevation consistent with the intersection of MB 139. Equation (49) for region Salado in Figure PA-8.

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Material	Property	Variable Name	Description
Name	Name		
S_HALITE	PRMX_LOG	HALPRM	Logarithm of intrinsic halite permeability (m2). Used in region Salado in Figure PA-8.
S_MB139	PORE_DIS	ANHBCEXP	Brooks-Corey pore distribution parameter for anhydrite (dimensionless). Equation (32) for regions MB 138, Anhydrite AB, and MB 139 of Figure PA-8 for use with Brooks-Corey model; Equations (36) for use with van Genuchten-Par
S_MB139	PRMX_LOG	ANHPRM	Logarithm of intrinsic anhydrite permeability (m2). Used in regions MB 138, Anhydrite AB, and MB 139 in Figure PA-8.
S_MB139	RELP_MOD	ANHBCVGP	Indicator for relative permeability model (dimensionless) for regions MB 138, Anhydrite AB and MB 139 in Figure PA-8. See Table PA-3.
S_MB139	SAT_RBRN	ANRBRSAT	Residual brine saturation in anhydrite (dimensionless). Defines Sbr in Equation (35) for regions MB 138, Anhydrite AB, and MB 139 in Figure PA-8.
SHFTL_T1	PRMX_LOG	SHLPRM2	Logarithm of intrinsic permeability (m2) of lower shaft seal materials for the first 200 years after closure. Used in region Lower Shaft in Figure PA-8.
SHFTL_T2	PRMX_LOG	SHLPRM3	Logarithm of intrinsic permeability (m2) of lower shaft seal materials from 200 years to 10,000 years after closure. Used in region Lower Shaft in Figure PA-8.
SHFTU	PRMX_LOG	SHUPRM	Logarithm of intrinsic permeability (m2) of upper shaft seal materials. Used in region Upper Shaft in Figure PA-8.
SHFTU	SAT_RBRN	SHURBRN	Residual brine saturation in upper shaft seal materials (dimensionless). Defines Sbr in Equation (35) for region Upper Shaft in Figure PA-8.
SHFTU	SAT_RGAS	SHURGAS	Residual gas saturation in upper shaft seal materials (dimensionless). Defines Sgr in Equation (34) for region Upper Shaft in Figure PA-8.
SOLMOD3	SOLVAR	WSOLVAR3	Solubility multiplier for +III oxidation states

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Material Name	Property Name	Variable Name	Description
SOLMOD4	SOLVAR	WSOLVAR4	Solubility multiplier for +IV oxidation states
SPALLMOD	PARTDIAM	SPPDIAM (previously SPLPTDIA, WPRTDIAM)	Particle diameter of disaggregated waste
SPALLMOD	REPIPERM	REPIPERM	Waste permeability of gas local to intrusion borehole.
SPALLMOD	REPIPOR	SPLRPOR	Waste porosity at time of drilling intrusion
SPALLMOD	TENSLSTR	TENSLSTR	Tensile strength of waste.
STEEL	CORRMCO2	WGRCOR	Rate of anoxic steel corrosion (m/s) under brine inundated conditions and with no CO2 present. Defines Rci in Equation (59) for areas Waste Panel, South RoR, and North RoR in Figure PA-8.
TH+4	MKD_TH	CMKDTH4	Matrix distribution coefficient (m3/kg) for Th in +4 oxidation state. Defines Kdk in Equation (231).
U+4	MKD_U	CMKDU4	Matrix distribution coefficient (m ³ /kg) for U in +4 oxidation state. Defines Kdk in Equation (231).
U+6	MKD_U	CMKDU6	Matrix distribution coefficient (m ³ /kg) for U in +6 oxidation state. Defines Kdk in Equation (231).
WAS_AREA	BIOGENFC	WBIOGENF	Probability of obtaining sampled microbial gas generation rates.
WAS_AREA	BRUCITEC	WBRUITEC	Waste emplacement area and waste,MgO inundated hydration rate in ERDA-6 brine
WAS_AREA	BRUCITEH	WBRUITEH	Waste emplacement area and waste,MgO humid hydration rate

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Material	Property	Variable Name	Description
Name	Name		
WAS_AREA	BRUCITES	WBRUITES	Waste emplacement area and waste,MgO inundated hydration rate in GWB brine
WAS_AREA	GRATMICH	WGRMICH	Rate of CPR biodegradation (mol C6H10O5 / kg C6H10O5 / s) under anaerobic, humid conditions. Defines Rmh in Equation (61) for areas Waste Panel, South RoR, and North RoR, in Figure PA-8.
WAS_AREA	GRATMICI	WGRMICI	Rate of CPR biodegradation (mol $C_6H_{10}O_5$ / kg $C_6H_{10}O_5$ / s) under anaerobic, brine-inundated conditions. Defines Rmi in Equation (61) for areas Waste Panel, South RoR, and North RoR, in Figure PA-8.
WAS_AREA	HYMAGCON	WHYMAGC	Waste emplacement area and waste,Rate of conversion of hydromagnesite to magnesite
WAS_AREA	PROBDEG	WMICDFLG	Index for model of microbial degradation of CPR materials (dimensionless). Used in areas Waste Panel, South RoR, and North RoR in Figure PA-8.
WAS_AREA	SAT_RBRN	WRBRNSAT	Residual brine saturation in waste (dimensionless). Defines Sbr in Equation (34) for areas Waste Panel, South RoR, and North RoR, in Figure PA-8; also used in waste material in Figure PA-20 for calculation of DBR; see Section PA-4.7.
WAS_AREA	SAT_RGAS	WRGSSAT	Residual gas saturation in waste (dimensionless). Defines Sgr in Equation (35) for areas Waste Panel, South RoR, and North RoR in Figure PA-8; also used in waste material in Figure PA-20 for calculation of DBR; see Section PA-4.7.
WAS_AREA	SAT_WICK	WASTWICK	Increase in brine saturation of waste due to capillary forces (dimensionless). Defines Swick in Equation (78) for areas Waste Panel, South RoR, and North RoR, in Figure PA_8.

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Changes from the PABC-2009

The changes implemented in the CRA-2014 analysis from the PABC-2009 analysis are documented in Camphouse (2013). These changes include updates of the inventory; changes in the configuration of the repository including the use of the "run of mine" salt panel closure system, the inclusion of additional mined region in the experimental area, and refinement in the water balance implementation; and changes in parameters based on new data including updated drilling parameters, the probability of hitting brine, waste shear strength, steel corrosion rate, and solubility multipliers. Overall, these changes reduced all releases at all probabilities (Figure 1).

Table 2. Parameters sampled by LHS having new distributions. The highlighted parameters were not sampled in the PABC-2009.

Material	Property
BOREHOLE	TAUFAIL
DRZ_PCS	RELP_MOD
GLOBAL	PBRINE
PCS_T1	PRMX_LOG
SOLMOD3	SOLVAR
SOLMOD4	SOLVAR
STEEL	CORRMCO2
WAS_AREA	BRUCITEC
WAS_AREA	BRUCITEH
WAS_AREA	BRUCITES
WAS_AREA	HYMAGCON

One hundred seventy-seven parameters were changed from their previous values and sixtysix new parameters were defined. Most of the distributions used for the CRA-2014 analysis were identical to those used in the PABC-2009. Ten sampled parameters were assigned new values, including six that had not been sampled in the PABC-2009 (Table 2). The distributions for the sampled parameters are reviewed in Kirchner (2013). The sensitivity analysis performed using stepwise regression cannot be used to explain sensitivity of the results to the changes implemented in the models, fixed parameters and inventory following the PABC-2009 analysis. The sensitivity analysis can only attempt to resolve the question of which *sampled* parameters contribute the most to the variability (uncertainty) observed in the mean releases by vector.

Limitations of the Analysis

Setting the STEPWISE parameter α_{out} to α_{in} maximizes the number of variables in the model (as requested by EPA in C-23-18, U.S. Environmental Protection Agency 2004) but can increase the number of spurious correlations (Kirchner 2004a, Kirchner 2004b). A spurious

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correlation implies a linear relationship exists between two variables but in reality no such relationship exists.

The STEPWISE procedure constructs a multivariate linear regression model. One of the assumptions of this statistical model is that the dependent (output) variable shows a linear response to the independent (input) variables. In cases where the response is non-linear but monotonic, replacing the values of the data with their ranks tends to linearize the response curves and standardizes the variability in the outputs and parameters by mapping the data into identical ranges. The rank of a value is an integer representing its position in the sorted list of the values. Ranking also tends to de-emphasize the impact of "outliers," which are points having considerably larger or smaller values than the remainder of the sample population. Although the use of ranks precludes using the model to predict values of an output variable given an input variable, the results are usually well suited for ranking the importance of the contributions of the input variables to the response of the output variable. The STEPWISE procedure has the functionality to perform ranked regressions. For the cases described below, the ranked regressions showed stronger correlations than the regressions based on the unranked data. This result suggests that there are non-linear relationships between the dependent and independent variables, but it does not eliminate the possibility that there are also non-monotonic relationships.

Ranked regression was used to evaluate the sensitivity of the output variables to the sampled parameters. Scatter plots of the dependent versus independent ranked variables resulting from the analysis were examined to determine if there were any obvious non-monotonic relationships. Obvious non-monotonic relationships were not found although there are cases involving inputs that are categorized as discrete variables (e.g. GLOBAL:OXSTAT, which is sampled as a uniform distribution but is then mapped to one of two discrete values). There are also cases (e.g. releases from the Culebra and spallings releases) where large proportions of the vectors in each replicate show no credible release values (values > 0.0001 EPA units) or zero releases (Tables 2 and 3). Values less than 0.0001 EPA units are considered to be dominated by numerical error and hence often unreliable. In terms of ranking the relative importance of the parameters the issue of a large proportion of zeros or unreliable values is most problematic.

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Release	Repl	Replicate 1		Replicate 2		Replicate 3	
	>0	≥0.0001	>0	≥0.0001	>0	≥0.0001	
Cuttings and Cavings	100	100	100	100	100	100	
Direct Brine	99	98	99	99	100	100	
Spallings	38	38	31	31	33	33	
Total	100	100	100	100	100	100	
Total From Culebra	95	18	94	19	98	11	
Total To Culebra	95	85	96	84	98	82	

	Table 3. Percentage	of vectors	whose maxima	exceed 0 and 0.00	01.
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Release	Repl	icate 1	Repl	icate 2	Replicate 3	
	>0	≥0.0001	>0	≥0.0001	>0	≥0.0001
Cuttings and Cavings	100	100	100	100	100	100
Direct Brine	99	74	99	81	100	69
Spallings	38	9	31	11	33	10
Total	100	100	100	100	100	100
Total From Culebra	95	6	94	8	98	6
Total To Culebra	95	67	96	72	98	67

Table 4. Percentage of vectors having non-zero mean releases and mean releases > 0.0001.

In general, the sensitivity of the vector means to the sampled parameters coupled with differences in the distribution of those parameters between analyses can be correlated with the observed differences between analyses in the mean CCDF curves for each type of release. For example, the distribution of a dominant parameter, BOREHOLE:TAUFAIL, was changed between the PABC-2009 and the CRA-2014 and corresponding changes can be seen in the mean CCDF curves for cuttings and cavings releases. However, changes in constant parameters and changes in the stochastic processes can also impact the means of the vectors. Thus, such correlations are not guaranteed and counterintuitive results are possible.

The mean and variance of the release for a given vector are controlled by the stochastic processes that govern the events in each future. A change in the frequency of a stochastic event such as drilling rate can shift a distribution left or right, thus changing the mean. However, changes that impact the shape of a distribution can also cause changes in the mean.

One potential disconnect between the sensitivity of the vector means to changes in the mean CCDF curves comes, in part, because the mean CCDF curves (Figure 1) are averages of the probabilities for a release, R, across vectors, $p_{R>x}$ at each release level x, i.e. for one replicate.

$$\overline{p}_{R>x} = \frac{1}{100} \sum_{1}^{100} p_{R>x}$$

In other words, the mean CCDF curves are created by averaging vertically the individual CCDF curves for the vectors (Figure 2). This is equivalent to pooling the data from all futures across vectors. The CCDF curves focus attention on the right tails of the distributions of releases rather than the vector means. The vector means, \overline{R}_{ν} are computed as the average of each release across the 10,000 futures, i.e.

$$\overline{R}_{\nu} = \frac{1}{10000} \sum_{i=1}^{10000} R_{\nu,i}$$

where $R_{v,i}$ is the release from the *i*th future of vector *v*. Thus one can imagine cases where the vector means for some type of release in one analysis are all greater than the corresponding

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vector means for that release in a second analysis and yet the CCDF curves for the vectors of the first analysis lie to the left of CCDF curves of the vectors of the second analysis. Figure 3A illustrates such a case with just one vector from two analyses. The mean of Analysis 1 exceeds the mean of Analysis 2 but because the variance of the distribution for Analysis 1 is smaller than the variance of the distribution for Analysis 2 (Fig. 3C) extends further to the right than the curve for Analysis 1.



Figure 1. Mean CCDFs across the replicates of the PABC-2009 analysis (dashed lines) and CRA-2014 PA analysis (solid lines).



Figure 2. CCDFs for individual vectors and the mean probability CCDF. Vector means are computed by averaging the releases from the 10,000 futures associated with each vector.

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Figure 3B illustrates a case where a change from a symmetric distribution (Analysis 3) to a right-skewed distribution (Analysis 4) causes an increase in the mean even though the modes remain the same. The CRA-2014 analysis had about a 12 % increase in the drilling rate, which is the primary determinant of the number of intrusion events into the repository. Thus some change in variability within vectors would be expected.





Most of the regression models produced by STEPWISE do not include all of the input variables, even after ranking the data. This simply indicates that the uncertainties in many of the parameters have statistically insignificant effects on the output variable. Statistical insignificance can arise because the output variable has a low functional response to the input variable, because the magnitude of uncertainty in the input variable is small relative to the other inputs, or from a combination of both conditions. This is not to say that these non-significant variables have no influence on the releases. Their exclusion from the tables reflects the inability of this statistical technique to rank their importance with an acceptable degree of confidence. For example, if the response of the output variable to an input variable

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was non-monotonic then the regression analysis might fail to properly identify that variable's importance. In addition, the stochastic processes modeled introduce variability that cannot be attributed to the sampled parameters so the regression analyses cannot be expected to explain all of the observed variability in the vector means. In the case of the WIPP releases the stochastic effects of drilling and mining intrusions (aleatory uncertainty) contribute to the variability in the release estimates. In the CRA-2014 65% to 72% of the variability in the total releases has been accounted for by the sampled input variables as measured by the R^2 value (coefficient of determination) (Table 5).

	Maximum Proportion of the Variance Accounted For By Stepwise Regression on Sampled Parameters									
Release	PABC-2009 Replicate 1	CRA-2014 Replicate 1	CRA-2014 Replicate 2	CRA-2014 Replicate 2						
Total	0.87	0.67	0.72	0.65						
Cuttings and Cavings	1.00	0.75	0.83	0.83						
Spallings	0.42	0.51	0.39	0.48						
Direct Brine	0.69	0.75	0.78	0.87						
From Culebra	0.71	0.73	0.73	0.61						
To Culebra	0.87	0.93	0.91	0.93						

Table 5. Maximum proportion of the variability in releases accounted for in stepwise rank regression.

Often several of the parameters that appear in the regression model contribute very little to the R^2 value and, therefore, explain very little of the variability in the output variable. Parameters that have minor contributions can appear by chance, simply due to random correlations. Many of the parameters that account for only a few percent to the variability in an output from one replicate may show different rankings, or can even be absent, in another replicate. Thus, it is difficult to assess the importance of the parameters that improve the regression model very little and, in reality, they may have no importance at all. Therefore, only the parameters that appear to have meaningful impacts on the regression model will be discussed.

Stepwise Results

In the tables below the cumulative R^2 value represents the proportion of total variation explained by the fitted regression using the listed variables, starting with the greatest contributor to the variance. The number of variables used in the regression model is determined by the stepwise regression procedure, as discussed above. Regression analyses are conducted for each replicate separately, with replicate 1 of the CRA-2014 PA being compared to replicate 1 of the PABC-2009 analysis.

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Total Releases

As in the PABC-2009 PA (Kirchner 2010), cuttings and cavings releases and direct brine releases account for the majority of the total releases estimated in the CRA-2014 (Figure 1). Releases from the Culebra contribute little to the total release except at low probabilities where, for the first time, they exceed releases from cuttings and cavings. This change is most likely due to the impact on Culebra releases of the changes in the distributions of SOLMOD3:SOLVAR, the variable representing model prediction error on the estimate of solubility of the +III state of actinides (Brush and Domski 2013) and the impact on cavings by the change in the distribution of waste shear strength BOREHOLE: TAUFAIL (Herrick and Kirchner 2013). Across the three replicates of the CRA-2014 65 % to 72 % of the variability is accounted for in the regression model containing the largest number of variables (Tables 6 and 7). The difference in the R^2 values for total releases between the CRA-2014 (67%) and the PABC-2009 PA (87%) reflects the changes in waste shear strength (BOREHOLE: TAUFAIL) (decreased in importance) and SOLMOD3: SOLVAR (increased in importance) (Table 6). In both analyses uncertainty in total releases is largely due to uncertainty in BOREHOLE: TAUFAIL. Two changes were made to the distribution of BOREHOLE: TAUFAIL; the lower bound was increased slightly and the distribution was assumed to be uniform whereas previously it was loguniform (Figure 4). These changes reduced the proportion of values at the low end of the range. Over 50% of the values sampled for the PABC-2009 fall below the lower limit of the range of BOREHOLE: TAUFAIL for the CRA-2014 analysis. The volumes of cavings are primarily controlled by shear strength, hence the negative correlation and the overall decrease in cuttings are expected. The decrease in importance of BOREHOLE: TAUFAIL appears to be related to a greater variability in the ranks of the total releases rather than a large change in the slope (Figure 5) although the slope did decrease. The increase in variability reflects the lower relative contribution of cuttings to total releases.



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Figure 4. Expected and observed distributions of BOREHOLE: TAUFAIL from the PABC-2009 and CRA-2014 analyses.



Figure 5. Simple correlation of total releases on waste shears strength for the PABC-2009 and the CRA-2014.

SOLMOD3:SOLVAR remained the second most dominant parameter contributing to variability in total releases in all three replicates. An update of the prediction error of the EQ3/6 model using data relevant to conditions in the WIPP repository (Brush and Domski 2013) increased the uncertainty on SOLMOD3:SOLVAR as compared to the PABC-2009 (Figure 6). SOLMOD3:SOLVAR is defined by a user-defined cumulative distribution. The lower bound was increased from -4.2 to about -3.5 and the upper bound from 2.7 to about 3.0. In addition, the CRA-2014 distribution is more platykutic (i.e. the PDF is less concentrated near the central tendency) than is the PABC-2009 distribution. SOLMOD3:SOLVAR not only accounts for prediction error of the EQ3/6 model but also corrects for bias in the baseline solubility of the +III actinides.

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CASTILER:PRESSURE is the initial brine pore pressure in the Castile. Solubility of actinides impacts their brine concentration and the initial pressure of that brine influences the volume of direct brine releases (DBR) and releases to the Culebra. CASTILER:PRESSURE is the third-ranked parameter of importance in the first two replicates but drops to sixth place in the third replicate. The third-ranked parameter in replicate 3 is GLOBAL:OXSTAT, the indicator variable for oxidation states of uranium and plutonium. Because GLOBAL:OXSTAT is used to switch between the +III and +IV oxidations states of uranium and plutonium it can impact releases, particularly direct brine releases. However, the composite variable OXSTAT is created to map GLOBAL:OXSTAT into a discrete Bernoulli distribution to match its impact on oxidation state exactly and yet composite:OXSTAT wasn't included in the analysis. Thus the correlation between total releases and GLOBAL:OXSTAT is likely to be spurious. This conclusion is reinforced by the absence of GLOBAL:OXSTAT in any other regression model in this analysis. The remaining parameters contribute only a few percent and thus are not important.

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	Expected Normalized Release								
	CRA-2014 Re		1	PABC-2009 Replicate 1					
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	R ²	SRRC			
1	BOREHOLE: TAUFAIL	0.33	-0.57	BOREHOLE:TAUFAIL	0.76	-0.88			
2	SOLMOD3:SOLVAR	0.47	0.38	SOLMOD3:SOLVAR	0.79	0.17			
3	CASTILER:PRESSURE	0.54	0.26	CELLULS:FBETA	0.81	-0.14			
4	S_HALITE:COMP_RCK	0.58	-0.18	CASTILER:PRESSURE	0.83	0.12			
5	SHFTU:SAT_RGAS	0.61	-0.17	GLOBAL:PBRINE	0.85	0.13			
6	WAS_AREA:PROBDEG	0.64	0.14	SHFTU:SAT_RGAS	0.85	-0.10			
7	S_HALITE:POROSITY	0.65	0.13	GLOBAL:TRANSIDX	0.86	0.09			
8	BOREHOLE:DOMEGA	0.67	0.13	BOREHOLE:DOMEGA	0.87	0.08			

 Table 6. Stepwise ranked regression analysis for mean Total releases, replicate 1 of the PABC-2009 and CRA-2014 analyses.

^a Steps in stepwise regression analysis b

^c Cumulative R² value with entry of each variable into regression model

b Variables listed in order of selection

d Standardized Rank Regression Coefficient

 Table 7. Stepwise ranked regression analysis for mean Total releases, replicates 2 and 3 of the CRA-2014 analysis.

	Expected Normalized Release									
	CRA-2014 Rep	CRA-2014 Replicate 2			CRA-2014 Replicate 3					
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	R ²	SRRC				
1	BOREHOLE:TAUFAIL	0.42	-0.64	BOREHOLE:TAUFAIL	0.32	-0.55				
2	SOLMOD3:SOLVAR	0.57	0.40	SOLMOD3:SOLVAR	0.43	0.32				
3	CASTILER:PRESSURE	0.61	0.25	GLOBAL:OXSTAT	0.50	0.25				
4	BOREHOLE:DOMEGA	0.63	0.15	BOREHOLE:DOMEGA	0.54	0.21				
5	WAS_AREA:PROBDEG	0.65	0.16	BH_SAND:PRMX_LOG	0.57	-0.19				
6	PCS_T1:PORE_DIS	0.68	-0.15	CASTILER:PRESSURE	0.60	0.18				
7	S_HALITE:POROSITY	0.69	0.13	S_HALITE:POROSITY	0.63	0.15				
8	WAS_AREA:SAT_RBRN	0.71	0.11	CULEBRA: APOROS	0.65	0.14				
9	CULEBRA:MINP_FAC	0.72	-0.11							

a Steps in stepwise regression analysis

^b Variables listed in order of selection

^c Cumulative R² value with entry of each variable into regression model

d Standardized Rank Regression Coefficient

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Cuttings and Cavings Releases

Tables 8 and 9 list the parameters that showed significant correlations to cuttings and cavings releases based on a stepwise regression using ranked data. Cutting and cavings releases are combined as outputs from CCDFGF because drilling intrusions produce both. Cuttings volume is controlled by the drill bit diameter whereas cavings volume depends on waste shear strength and, to a much smaller extent, the angular velocity of the drill string (BOREHOLE:DOMEGA) as is discussed in Dunagan (2004) and Ismail and Garner (2010). The uncertainty in mean cuttings and cavings releases is primarily due to the uncertainty in the cuttings and cavings volume. Waste shear strength (BOREHOLE: TAUFAIL) controls about 65 % of the variability in mean cuttings and cavings releases in replicate 1 of the CRA-2014 PA as compared to 98 % in replicate 1 of the PABC-2009. This difference is undoubtedly due to the change in the distribution of BOREHOLE: TAUFAIL from a loguniform distribution to a uniform distribution of somewhat smaller (< 3 %) range (Herrick and Kirchner 2013). Even the logarithms of cuttings and cavings releases exhibit non-linear behavior to the logarithms of BOREHOLE: TAUFAIL (Figure 7). Figure 7 also shows that the variability of the CCDFs for cuttings and cavings is impacted by the magnitude of BOREHOLE: TAUFAIL even though the variability is controlled by stochastic processes (drilling events). Both the mean and the variability of cuttings depend on BOREHOLE: TAUFAIL because it is a threshold controlling whether an event will create cavings; larger values mean fewer cavings events hence lower means and less dispersion around the mean. The remaining parameters in Tables 8 and 9 explain less than about 1 % of the variability in cuttings and cavings and are undoubtedly spurious since they have no functional influence on cuttings and cavings.

Table 8. Stepwise ranked regression analysis for mean Cuttings and Cavings releases, replicate 1 of th	e
PABC-2009 and CRA-2014 analyses.	

	Expected Normalized Release									
	CRA-2014 R	eplicate	1	PABC-2009 R	eplicate	1				
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	\mathbf{R}^2	SRRC				
1	BOREHOLE:TAUFAIL	0.65	-0.82	BOREHOLE:TAUFAIL	0.98	-0.99				
2	BOREHOLE:DOMEGA	0.72	0.25	BOREHOLE:DOMEGA	1.00	0.11				
3	(Composite):MKD_U	0.74	-0.16	SHFTL_T1:PRMX_LOG	1.00	0.02				
4	SHFTU:SAT_RBRN	0.75	0.11	(Composite):OXSTAT	1.00	-0.02				
5				CULEBRA:HMBLKLT	1.00	0.02				
6				DRZ_PCS:PRMX_LOG	1.00	0.01				

^a Steps in stepwise regression analysis

^b Variables listed in order of selection

^c Cumulative R² value with entry of each variable into regression model

^d Standardized Rank Regression Coefficient

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		Exp	ected Nor	rmalized Release			
	CRA-2014 Rep	olicate		CRA-2014 Replicate 3			
Step ^a	Variable ^b	R ^{2c}		Variable	\mathbf{R}^2	SRRC	
1	BOREHOLE:TAUFAIL	0.72	-0.84	BOREHOLE:TAUFAIL	0.65	-0.79	
2	BOREHOLE:DOMEGA	0.78	0.26	BOREHOLE:DOMEGA	0.73	0.31	
3	PCS_T2:POR2PERM	0.81	0.18	CULEBRA: APOROS	0.75	0.12	
4	PHUMOX3:PHUMCIM	0.82	-0.10	S_HALITE:POROSITY	0.77	0.11	
5	CASTILER:PRMX_LOG	0.83	0.09	S_MB139:SAT_RBRN	0.78	-0.10	
6				SHFTU:SAT_RBRN	0.79	-0.11	
7				SOLMOD4:SOLVAR	0.80	-0.10	
8				SPALLMOD:REPIPERM	0.81	0.10	
9				WAS_AREA:BRUCITEH	0.82	0.09	
10				(Composite):OXSTAT	0.83	0.09	

Table 9. Stepwise ranked regression analysis for mean Cuttings and Cavings releases, replicates 2 and 3 of the CRA-2014 analysis.

^a Steps in stepwise regression analysis

b Variables listed in order of selection

^c Cumulative R² value with entry of each variable into regression model

d Standardized Rank Regression Coefficient

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Figure 7. The volume of cuttings and cavings (A), releases from cuttings and cavings (B) and the standard deviations of cuttings and cavings (C).

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Spallings Releases

Spallings releases are controlled by the spallings volume releases and the concentration of radionuclides in the waste streams encountered by drilling intrusions. Spalling volume releases are controlled by gas pressures in the repository, which must exceed a threshold of 8 MPa to occur, and the sampled parameters SPALLMOD: PARTDIAM (the particle diameter for disaggregated waste), SPALLMOD:REPIPOR (waste porosity), SPALLMOD: REPIPERM (waste permeability) and SPALLMOD: TENSLSTR (tensile strength of the waste). The distributions of the sampled parameters are the same as in the PABC-2009 analysis. The CRA-2014 spallings release volumes decreased from the PABC-2009 analysis levels (Fig. 8). The spallings releases for CRA-2014 were smaller than those of the PABC-2009 as well (Fig. 9). Across replicates, the number of vectors having spallings releases in the CRA-2014 that exceeded 0.0001 was just 2 vectors fewer than in the PABC-2009. The number of zero-releases (Table 2) was high enough to reduce the effectiveness of the regression analysis. A large number of zero values in the data tend to negate the assumption of linear regression that errors (residuals) are normally distributed. In addition, the distribution of zeros along the independent axis can exert a lot of control on the slope of the regression model.

Table 10 compares the parameters that showed correlation to mean spallings releases after a stepwise ranked regression using data from replicate 1 of the CRA-2014 and PABC-2009 analyses. The dominant parameter with regard to controlling spallings releases in the PABC-2009 assessment is S HALITE: POROSITY, the effective porosity of intact halite. The positive correlation is likely to be due to having greater gas pressures under higher porosities due to greater brine flow into the repository. S HALITE: POROSITY comes into the regression model in the fourth and second steps of replicates 2 and 3, respectively, but does not enter the regression model at all in replicate 1. The dominant parameter in replicates 1 and 3 of the CRA-2014 PA is SPALLMOD: PARTDIAM. SPALLMOD: PARTDIAM is ranked third in replicate 2. A negative correlation is observed in all of the regression models (Figure 10). The negative correlation with SPALLMOD:PARTDIAM is probably due to the tendency to have greater fluidization at smaller particle diameters. BH SAND:PRMX LOG is ranked second in replicates 1 and 2 and sixth in replicate 3 of the CRA-2014 PA. CASTILER: PRESSURE is ranked within the top three parameters in all three replicates and is the dominant parameter in the second replicate. CASTILER:PRESSURE is the initial brine pore pressure in the Castile and hence impacts brine intrusions into the repository. BH SAND:PRMX LOG is the log of the intrinsic permeability of a borehole filled with silty sand. Although defined for the "X" direction, the permeabilities for the Y and Z directions are assigned the same values as those sampled for the X direction. These parameters influence spallings releases by their impact on repository pressures. The remaining variables contribute only a few percent each to the total variability and the ranking of their importance to determining spallings releases is thus questionable.

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Figure 8. Mean Spalling volumes across all three replicates from the PABC-2009 and CRA-2014 analyses.



Figure 9. Mean Spalling releases across all three replicates from the PABC-2009 and CRA-2014 analyses.

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	Expected Normalized Release								
	CRA-2014 Rep	1	PABC-2009 Replicate 1						
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	R ²	SRRC			
1	SPALLMOD:PARTDIAM	0.11	-0.35	S_HALITE:POROSITY	0.14	0.34			
2	BH_SAND:PRMX_LOG	0.22	-0.33	SPALLMOD:PARTDIAM	0.22	-0.28			
3	CASTILER:PRESSURE	0.32	0.35	CULEBRA:DPOROS	0.26	-0.23			
4	SPALLMOD:REPIPOR	0.36	-0.21	CASTILER:PRESSURE	0.30	0.19			
5	WAS_AREA:PROBDEG	0.40	0.21	SHFTL_T2:PRMX_LOG	0.33	-0.18			
6	PCS_T3:POROSITY	0.43	0.18	WAS_AREA:PROBDEG	0.36	0.17			
7	WAS_AREA:BIOGENFC	0.45	0.18	DRZ_PCS:PRMX_LOG	0.39	-0.18			
8	S_MB139:RELP_MOD	0.48	-0.19	S_MB139:PRMX_LOG	0.42	0.16			
9	SHFTU:SAT_RGAS	0.51	0.16						

Table 10. Stepwise ranked regression analysis for mean Spallings releases, replicate 1 for the CRA-2014 and PABC-2009 analyses.

a Steps in stepwise regression analysis

^c Cumulative R² value with entry of each variable into regression model
 ^d Standardized Rank Regression Coefficient

b Variables listed in order of selection

Table 11. Stepwise ranked regression analysis for mean Spallings releases, replicates 2 and 3 of the CRA-2014 analysis.

	Expected Normalized Release										
	CRA-2014 Re		2	CRA-2014 Rep	licate	3					
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	\mathbf{R}^2	SRRC					
1	CASTILER:PRESSURE	0.12	0.35	SPALLMOD:PARTDIAM	0.11	-0.29					
2	BH_SAND:PRMX_LOG	0.22	-0.32	S_HALITE:POROSITY	0.21	0.32					
3	SPALLMOD:PARTDIAM	0.26	-0.20	CASTILER:PRESSURE	0.28	0.28					
4	S_HALITE:POROSITY	0.30	0.21	DRZ_PCS:PRMX_LOG	0.33	-0.22					
5	WAS_AREA:SAT_WICK	0.33	0.20	SPALLMOD:TENSLSTR	0.38	-0.21					
6	WAS_AREA:BIOGENFC	0.36	0.18	BH_SAND:PRMX_LOG	0.42	-0.22					
7	BOREHOLE:DOMEGA	0.39	-0.17	WAS_AREA:PROBDEG	0.45	0.17					
8				SHFTU:PRMX_LOG	0.48	0.16					

a Steps in stepwise regression analysis

b Variables listed in order of selection

^c Cumulative R² value with entry of each variable into regression model

d Standardized Rank Regression Coefficient

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Figure 10. Non-zero spallings release shows a negative correlation (p < 0.01) with SPALLMOD:PARTDIAM.

Direct Brine Release

Direct brine releases (DBR) are releases of contaminated brine originating in the repository and flowing up an intrusion borehole during the period of drilling and before the hole is plugged. In order for DBR to occur volume-averaged pressure near the borehole must exceed 8 MPa and brine saturation in the repository must exceed the residual saturation of the waste material (Malama 2013). The magnitudes of the releases depend on the volume of the release and the concentration of radionuclides within the brine. The CRA-2014 analysis shows a decrease in DBR as compared to the PABC-2009 analysis (Figure 11). The PABC-2009 analysis shows that four variables (SOLMOD3:SOLVAR, CASTILER:PRESSURE, STEEL:CORRMCO2 and GLOBAL:PBRINE) account for more than 50 % of the uncertainty in DBR (Table 12). SOLMOD3:SOLVAR and CASTILER:PRESSURE are ranked first and second in importance, respectively, in all three replicates of the CRA-2014 (Tables 12 and 13). However, in the CRA-2014 STEEL:CORRMCO2 did not enter the regression model for any replicate and GLOBAL:PBRINE enter the regression models of replicates 2 and 3 only in steps 5 and 13, respectively. This reduction in importance for GLOBAL:PBRINE and STEEL:CORRMCO2 is most likely related to the reduction in the ranges of the distributions assigned to these two parameters based on an analysis of

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additional drilling data in the area surrounding the WIPP (Kirchner, Kirkes and Zeitler 2013) and new experimental data (Roselle 2013), respectively. An increase in brine volume releases occurred as a result of changes in the panel closure system, drilling rates and plugging patterns as can be seen in the comparison of the Baseline (BL) case to PABC-2009 (Figure 12). In that figure the BL case represents the baseline changes, i.e. changes in the panel closure system, inclusion of the additional mined region in the experimental area, the updated inventory and updated drilling rate and plugging pattern parameters (Camphouse 2013). The TP case represents the baseline case with the inclusion of the new BOREHOLE: TAUFAIL (which does not impact DBR) and GLOBAL:PBRINE parameters, while the CRA-2014 case adds the implementation of variable brine volumes, refinements in the water balance calculations and the update of STEEL:CORRMCO2. The change in the distribution of GLOBAL:PBRINE reduced brine volumes at probabilities greater than 0.01 but had little impact on lower probability, higher volume releases. The addition of changes in the distribution of STEEL:CORRMCO2, which reduced pressures in the repository, is reflected in the line labeled CRA-2014. The net effect of all changes since the PABC-2009 was to reduce the probability of a direct brine volume release for volumes greater than 0.0001 m³ by about 33 % over much of that range.

The factors impacting direct brine releases, in addition to changes in the volume of the releases, are those that control the concentration of radionuclides in the brine, i.e. the sampled parameters SOLMOD3:SOLVAR for +III actinides and SOLMOD4:SOLVAR for +IV actinides. SOLMOD3:SOLVAR represents a distribution of EQ3/6 model prediction error on the estimate of solubility of the +III state of actinides. EQ 3/6 is used to estimate the radionuclide concentrations under WIPP repository conditions. The uncertainty in the predictions for the +III actinides is represented by multiplying the baseline solubility values by values sampled from the SOLMOD3:SOLVAR distribution. The distribution is constructed from the ratio of experimentally observed concentrations taken from the literature to EQ3/6 predictions based on the experimental conditions. This approach not only accounts for model prediction error but also introduces a correction for model bias, i.e. the mean ratio of observed to predicted. The same method is used to construct and employ the distribution of SOLMOD4:SOLVAR.

SOLMOD3:SOLVAR is the dominant sampled parameter controlling direct brine releases in all three CRA-2014 replicates, and it accounts for 36 % to 57 % of the observed variability in DBR. This is a greater proportion than that observed in the PABC-2009 analysis for DBR and is undoubtedly due to an increase in the variability of SOLMOD3:SOLVAR due to a new analysis of the literature data (Brush and Domski 2013). One feature of this new analysis was to make the distributions of prediction error more representative of WIPP conditions by selecting experimental results which were derived from brines similar in composition to those found in WIPP. The mean of the distribution changed from 0.07 (increasing the baseline solubility) to -0.68 (reducing the mean solubility). The impact of the change come not from reducing the mean solubility but from increasing the variance and making the distribution more platykurtic, i.e. more evenly distributed over the range.

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SOLMOD4:SOLVAR was included in the regression models for the three replicates in steps 10, 3 and 6, respectively. It accounts for only 1% to 4% of the variability. The variance of SOLMOD4:SOLVAR was reduced from that used in the PABC-2009 analysis, although the mean was increased from -0.52 (reducing the baseline solubility) to 0.66 (increasing the baseline solubility).

CASTILER:PRESSURE, the second most dominant parameter, is the initial brine pore pressure in the Castile. CASTILER:PRESSURE and GLOBAL:PBRINE control the frequency with which Castile brine intrudes the repository due to a drilling event and the initial pressure of that brine, thus their positive correlation with DBR is expected.

The remaining parameters contribute only a few percent each to explaining the variability in DBR. Many of these can be associated with their influence on gas pressures in the repository, For example, S_HALITE:POROSITY is the effective porosity in intact halite. The positive correlation is likely to be due to having greater gas pressures under higher porosities due to greater brine flow into the repository. BH_SAND:PRMX_LOG is the log of the intrinsic permeability of a borehole filled with silty sand. WAS_AREA:PROBDEG is the probability of microbial degradation of CPR materials, with a 75 % chance of degrading only cellulose and a 25 % chance of degrading cellulose, plastic and rubber. Microbial degradation generates gas in the repository. WAS_AREA:BIOGENFC is the probability of attaining the sampled microbial gas generation rate and reflects the uncertainty of whether 1) microbes will survive a significant fraction of the 10,000 year regulatory period, 2) whether water will be present, 3) whether CPR will be present, 4) whether electron receptors will be available, and 5) whether sufficient nutrients will be available (Nemer et al. 2005). S_MB139:RELPMOD is used to represent model uncertainty in a BRAGFLO process, selecting between one of two different relative permeability models.

S_HALITE:COMP_RCK is the bulk compressibility of intact halite. The remaining parameters enter the regression model of only one of the three replicates, hence are probably of no importance.

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Figure 11. Mean Direct Brine Releases for the PABC-2009 and CRA-2014 analyses.



Figure 12. Comparison of mean CCDF curves for brine volume releases.

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	Expected Normalized Release								
	CRA-2014 Replicate 1			PABC-2009 Replicate 1					
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	\mathbf{R}^2	SRRC			
1	SOLMOD3:SOLVAR	0.36	0.59	SOLMOD3:SOLVAR	0.19	0.42			
2	CASTILER:PRESSURE	0.54	0.44	CASTILER:PRESSURE	0.35	0.40			
3	WAS_AREA:PROBDE G	0.58	0.22	GLOBAL:PBRINE	0.45	0.33			
4	WAS_AREA:BIOGENF C	0.62	0.21	STEEL:CORRMCO2	0.55	-0.30			
5	BH_SAND:PRMX_LOG	0.65	-0.19	S_MB139:RELP_MOD	0.58	-0.18			
6	S_HALITE:POROSITY	0.68	0.15	WAS_AREA:BIOGENFC	0.60	0.15			
7	S_MB139:RELP_MOD	0.70	-0.16	S_HALITE:POROSITY	0.63	0.15			
8	S_HALITE:COMP_RC K	0.71	-0.13	CONC_PCS:SAT_RGAS	0.65	-0.14			
9	(Composite):OXSTAT	0.73	0.14	S_MB139:PRMX_LOG	0.67	0.14			
10	SOLMOD4:SOLVAR	0.74	0.11	WAS_AREA:SAT_WICK	0.69	-0.14			
11	GLOBAL:CLIMTIDX	0.75	-0.11						

Table 12. Stepwise ranked regression analysis for mean Direct Brine releases of the CRA-2014 a	ınd
PABC-2009 analyses.	

^a Steps in stepwise regression analysis

b Variables listed in order of selection

^c Cumulative R² value with entry of each variable into regression model ^d Standardized Rank Regression Coefficient

Table 13. Stepwise ranked regression analysis for mean Direct Brine releases, replicates 2 and 3 of the CRA-2014 analysis.

	Expected Normalized Release									
	CRA-2014 Replicate 2			CRA-2014 Replicate 3						
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	\mathbf{R}^2	SRRC				
1	SOLMOD3:SOLVAR	0.57	0.78	SOLMOD3:SOLVAR	0.46	0.63				
2	CASTILER:PRESSURE	0.63	0.24	CASTILER:PRESSURE	0.64	0.42				
3	SOLMOD4:SOLVAR	0.67	0.21	BH_SAND:PRMX_LOG	0.72	-0.29				
4	BH_SAND:PRMX_LOG	0.71	-0.20	DRZ_1:PRMX_LOG	0.76	-0.18				
5	GLOBAL:PBRINE	0.73	0.15	S_HALITE:POROSITY	0.78	0.12				
6	S_HALITE:POROSITY	0.74	0.13	SOLMOD4:SOLVAR	0.80	0.15				
7	SPALLMOD:REPIPOR	0.76	0.13	(Composite):MKD_U	0.81	-0.13				

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Sensitivity of CRA-2014 PA Releases to Parameters

	Expected Normalized Release								
	CRA-2014 Replicate 2			CRA-2014 Replicate 3					
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	\mathbf{R}^2	SRRC			
8	CASTILER:COMP_RCK	0.78	0.12	S_HALITE:COMP_RCK	0.83	-0.13			
9				DRZ_PCS:PRMX_LOG	0.84	-0.11			
10				WAS_AREA:SAT_RBRN	0.85	-0.09			
11				S_MB139:RELP_MOD	0.86	-0.09			
12				CULEBRA:MINP_FAC	0.86	0.08			
13			1	GLOBAL:PBRINE	0.87	0.08			

a Steps in stepwise regression analysis
 b Variables listed in order of selection

^c Cumulative R^2 value with entry of each variable into regression model

^d Standardized Rank Regression Coefficient

Culebra Releases

The release of radionuclides from the Culebra starts with the transport of the radionuclides to the Culebra. A regression analysis on the non-zero data shows that the logarithms of these two releases are well correlated although the scatter of residuals is still quite large ($R^2 = 0.52$, Figure 13).



Figure 13. Correlation between releases to and from the Culebra.

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Sensitivity of CRA-2014 PA Releases to Parameters

The CCDF for mean probabilities *from* the Culebra showed a decrease in the upper tail between the PABC-2009 and the CRA-2014 PA (Fig. 1). The decrease in the mean probability for releases > 0.001 EPA unit can result from having a greater proportion of vectors with zero releases, reduced levels of releases, lower variability within vectors, a change in skewness or a combination of these factors. The releases of zero are due, for the most part, to transport rates frequently being too small to enable contaminants to reach the boundary within the simulation period, 10,000 years. The times of the intrusions giving rise to flows to the Culebra are also likely to influence whether or not such releases occur. These times are not represented in the "sampled" input parameters and thus cannot be associated with the releases in a sensitivity analysis. Changes in the releases from the Culebra are not due to changes in the rate of transport because 1) the flow fields used in the CRA-2014 analysis were the same as those used in the PABC-2009 analysis, and 2) there were no changes in the matrix distribution coefficients (K_d) for the radionuclides, so there was no change in the retardation during transport. The increase in the drilling rate may have caused some vectors to have releases whereas previously that had none because of having earlier intrusion times in some futures, thus providing the time needed to have the radionuclides reach the land withdrawal boundary. In the PABC-2009 the percentages of the vectors for replicates 1, 2 and 3 having zero releases were 9 %, 7 % and 6 respectively. In the CRA-2014 these percentages were 5%, 6% and 2%. However, in both analyses the same thirtytwo vectors across the three replicates had releases exceeding 0.0001 EPA units.

The distribution of the means by vector shows a shift toward somewhat larger release values, although most vectors have means well below the 0.0001 EPA unit that is generally considered credible in terms of numerical computational error (Fig. 14). These histograms may seem at odds with the mean CCDF curves for releases from the Culebra in Figure 1, but Figure 1 is plotting mean probabilities across vectors (i.e. data in Figure 15 are averaged vertically), whereas Figure 14 is plotting the means by vector (i.e. the mean of each CCDF curve in Figure 15 as well as those not displayed because their curves never exceeded 0.0001 EPA unit). Vertical averaging results in fewer and fewer vectors with non-zero probabilities at a given release going into the calculation of the mean probability as release value increases. Therefore, the curve of mean probabilities as the release level increases is influenced more and more by the shape of the CCDF curves for individual vectors that remain above zero until only one vector controls the shape of the mean value curve. In other words, the sensitivity analysis shows the impact of parameters on the mean of the distributions associated with each vector but about 90% of those curves terminate (go to zero) at release below 0.0001 EPA units and hence the sensitivity analysis may do little to help explain the behavior of the curve for mean probability of release from the Culebra shown in Figure 1.

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Figure 14. Mean releases from the Culebra by vector across replicates. The vertical line is at 0.0001 EPA unit.



Figure 15. Releases from the Culebra by vector.

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A dominant parameter in the CRA-2009 PA analysis of releases both to the Culebra and from the Culebra is BH SAND: PRMX LOG, the logarithm of intrinsic permeability in the Xdirection for a sand-filled borehole (Tables 12, 13, 14 and 15). Conceptually, the flow of brine up the borehole (and thus to the Culebra) should be positively influenced by increasing values for BH SAND:PRMX LOG (Stein and Zelinski 2003). This parameter accounts for 27 % to 42 % of the variability in releases from the Culebra and 82 % to 85 % of the releases to the Culebra across the three replicates of the CRA-2014. Composite: MKD U was the dominant parameter in replicate 1 of releases from the Culebra. It was also ranked sixth in replicate 2 and second in replicate 3 of releases from the Culebra. The negative correlation between Culebra releases and Composite:MKD U was expected because high values of K_d suppress the transport of the radionuclide. Although SOLMOD3:SOLVAR is ranked second in all three replicates of the releases to the Culebra, it only appears in replicate 1 at rank 6 in releases from the Culebra. Similarly, CASTILER: PRESSURE is ranked third in all three replicates of releases to the Culebra, but is not included in any of the regression models for releases from the Culebra. CASTILER:PRESSURE is the initial brine pore pressure in the Castile brine reservoir and thus controls brine flow into the repository from an intrusion into a brine pocket. SOLMOD3:SOLVAR explains no more than 6 % of the variability in releases to the Culebra, and CASTILER:PRESSURE explains only 1 %.

	Expected Normalized Release							
	CRA-2014 Rep	1	PABC-2009 Replicate 1					
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	\mathbf{R}^2	SRRC		
1	(Composite):MKD_U	0.39	-0.41	BH_SAND:PRMX_LOG	0.46	0.63		
2	BH_SAND:PRMX_LOG	0.54	0.42	(Composite):MKD_U	0.58	-0.36		
3	CULEBRA: APOROS	0.58	-0.17	DRZ_PCS:PRMX_LOG	0.61	0.17		
4	GLOBAL:CLIMTIDX	0.61	0.18	SOLMOD4:SOLVAR	0.63	-0.17		
5	CULEBRA:HMBLKLT	0.64	0.19	CULEBRA:HMBLKLT	0.65	0.16		
6	SOLMOD3:SOLVAR	0.66	0.14	CULEBRA: APOROS	0.67	-0.14		
7	DRZ_PCS:PRMX_LOG	0.67	0.16	(Composite):MKD_PU	0.69	-0.14		
8	WAS_AREA:SAT_WICK	0.69	0.13	STEEL:CORRMCO2	0.71	-0.13		
9	(Composite):MKD_PU	0.70	-0.13					
10	(Composite):OXSTAT	0.72	0.18					
11	S_HALITE:POROSITY	0.73	-0.11					

 Table 12. Stepwise ranked regression analysis for mean releases from the Culebra for the CRA-2014 and PABC-2009 analyses.

^a Steps in stepwise regression analysis

b Variables listed in order of selection

^c Cumulative R² value with entry of each variable into regression model

¹ Standardized Rank Regression Coefficient

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Step ^a	Expected Normalized Release							
	CRA-2014 Replicate 2			CRA-2014 Replicate 3				
	Variable ^b	R ^{2c}	SRRC ^d	Variable	\mathbf{R}^2	SRRC		
1	BH_SAND:PRMX_LOG	0.42	0.59	BH_SAND:PRMX_LOG	0.27	0.49		
2	(Composite):OXSTAT	0.59	0.33	(Composite):MKD_U	0.44	-0.42		
3	CULEBRA:MINP_FAC	0.64	-0.19	CULEBRA: APOROS	0.57	-0.37		
4	CULEBRA:HMBLKLT	0.66	0.16	PCS_T1:SAT_RBRN	0.59	-0.14		
5	CULEBRA: APOROS	0.68	-0.14	PCS_T1:POROSITY	0.61	0.14		
6	(Composite):MKD_U	0.70	-0.19					
7	SHFTU:SAT_RGAS	0.71	-0.13					
8	WAS AREA:GRATMICH	0.73	-0.12					

 Table 13. Stepwise ranked regression analysis for mean releases from the Culebra, replicates 2 and 3 of the CRA-2014 analysis.

^b Variables listed in order of selection

^c Cumulative R² value with entry of each variable into regression model ^d Standardized Rank Regression Coefficient

CULEBRA:APOROS is the only other parameter that appears in all three regression models for the CRA-2014 releases from the Culebra. CULEBRA:APOROS is the Culebra advective porosity (the fracture volume per unit volume of porous media) and is ranked third in the regression models for replicate 1 and 3 and fifth in the model for replicate 2. Negative correlations are expected for this variable because it affects the velocity of transport. Low porosities increase the rate of transport as compared to high porosities and hence increase the likelihood of a release at the Land Withdrawl Boundary within 10,000 years. The remaining parameters for the regression models for releases from the Culebra each only explain a few percent of the variability. For releases to the Culebra, SOLMOD4:SOLVAR is the only remaining parameter found in all three regression models for the CRA-2014 analysis and it explains no more than 1 % of the variability. The remaining parameters each explain no more than a few percent of the variability in the releases.

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	Expected Normalized Release							
	CRA-2014 Replicate 1			PABC-2009 Replicate 1				
Step ^a	Variable ^b	R ^{2c}	SRRC ^d	Variable	\mathbf{R}^2	SRRC		
1	BH_SAND:PRMX_LOG	0.83	0.90	BH_SAND:PRMX_LOG	0.80	0.91		
2	SOLMOD3:SOLVAR	0.88	0.23	STEEL:CORRMCO2	0.82	-0.15		
3	CASTILER:PRESSURE	0.89	0.10	DRZ_PCS:PRMX_LOG	0.84	0.13		
4	DRZ_PCS:PRMX_LOG	0.90	0.09	CASTILER:PRESSURE	0.84	0.08		
5	WAS_AREA:PROBDEG	0.90	0.08	SOLMOD3:SOLVAR	0.85	0.10		
6	GLOBAL:OXSTAT	0.91	0.07	(Composite):MKD_U	0.86	0.08		
7	SOLMOD4:SOLVAR	0.91	0.07	SOLMOD4:SOLVAR	0.86	-0.08		
8	CULEBRA:HMBLKLT	0.92	0.06	GLOBAL:TRANSIDX	0.87	0.08		
9	S_HALITE:COMP_RCK	0.92	0.45					
10	S_HALITE:PRMX_LOG	0.93	0.39					

 Table 14. Stepwise ranked regression analysis for mean releases to Culebra, replicate 1 for the CRA-2014 and PABC-2009 analyses.

^a Steps in stepwise regression analysis

^c Cumulative R² value with entry of each variable into regression model

b Variables listed in order of selection

d Standardized Rank Regression Coefficient

Table 15. Stepwise ranked regression analysis for mean releases to Culebra, replicates 2 and 3 of the CRA-2014 analysis.

Step ^a	Expected Normalized Release							
	CRA-2014 Re	plicate	2	CRA-2014 Replicate 3				
	Variable ^b	R ^{2c}	SRRC ^d	Variable	R ²	SRRC		
1	BH_SAND:PRMX_LOG	0.85	0.92	BH_SAND:PRMX_LOG	0.82	0.91		
2	SOLMOD3:SOLVAR	0.89	0.23	SOLMOD3:SOLVAR	0.88	0.24		
3	CASTILER:PRESSURE	0.90	0.10	CASTILER:PRESSURE	0.89	0.11		
4	(Composite):OXSTAT	0.91	0.08	SOLMOD4:SOLVAR	0.90	0.09		
5	SOLMOD4:SOLVAR	0.91	0.07	WAS_AREA:BRUCITEC	0.91	-0.08		
6				GLOBAL:OXSTAT	0.91	0.08		
7				WAS_AREA:SAT_RGAS	0.92	0.07		
8				S_HALITE:POROSITY	0.92	-0.07		
9				GLOBAL:TRANSIDX	0.93	0.06		

^a Steps in stepwise regression analysis

^c Cumulative R² value with entry of each variable into regression model

^b Variables listed in order of selection

d Standardized Rank Regression Coefficient

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Dispersion versus Central Tendency

This analysis focusses on the impact of uncertainty in model parameters on the model outputs where the central tendency as measured by the mean of each vector is used at the dependent variable. However, the CCDFs of an output can also be characterized by their dispersion, typically expressed as the variance or standard deviation of the distributions. This question could be addressed using stepwise regression of the standard deviations against the sampled parameters. However, regression of the standard deviations against the means of the vectors for the releases show that, in general, the standard deviations are significantly (p<0.0001) correlated with the means (Figures 16 to 20). Log-log plots were used as needed to show the data where it covered several orders of magnitude. Because of these correlations, a separate set of regression analyses of standard deviations against parameter values would show few substantive differences. The variability in the residuals in the graph for total releases (Figure 16) reflects the addition of the two highly variable but uncorrelated components that contribute most to total releases, cuttings and cavings and direct brine releases (Figure 21).



Figure 16. Standard deviation versus the mean for total releases.

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Figure 17. Standard deviation versus the mean for cutting and cavings releases.



Figure 18. Standard deviation versus the mean for spallings releases.

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Figure 19. Standard deviation versus the mean for DBR releases.



Figure 20. Standard deviation versus the mean for releases from the Culebra.

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Summary and Conclusions

Cuttings and caving releases remain the primary contributor to total releases at the highest probabilities, with DBR becoming more important at low probabilities. BOREHOLE:TAUFAIL controls about 65 % to 72 % of the variability in mean cuttings and cavings releases through its highly non-linear relationship with the volume of cuttings and cavings produced. In the PABC-2009 analysis BOREHOLE:TAUFAIL explained about 98 % of the variability in cuttings and cavings releases. The decrease in the importance in BOREHOLE:TAUFAIL is undoubtedly due to the increase in the minimum of its distribution.

Spallings were reduced in the CRA-2014 analysis as compared to the PABC-2009 analysis with a reduction in repository gas pressure being the most likely cause. In terms of the sampled parameters, changes to the STEEL:CORRMCO2 distribution were responsible for much of the change in gas pressures, although changes in the configuration of the repository also had an impact. SOLMOD3:SOLVAR explains more of the variability in total releases in the CRA-2014 than it did in the PABC-2009, most likely because the range on the prediction error that it represents increased due to new data being added to the analysis of the EQ3/6 model.

Of the other parameters that were changed or were new since the PABC-2009 (Table 2), none had any substantial impact on releases. The influence of GLOBAL:PBRINE on DBR was somewhat reduced in comparison to the PABC-2009. The change in the distribution of

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SOLMOD4:SOLVAR had little impact on DBR or releases from the Culebra. Neither DRZ_PCS:RELP_MOD, PCS_T1:PRMX_LOG, WAS_AREA:BRUCITES nor WAS_AREA:HYNAGCON showed any correlation with releases from the repository, and WAS_AREA_BRUCITEC and WAS_AREA_BRUCITEH showed only very weak and inconsistent correlations with releases to the Culebra and cuttings and cavings, respectively.

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Attachment 1. CD containing the CCDFGF_Analysis.mdb and CCDFGF_Data.mdb databases

The attached CD contains copies of the CCDFGF_Analysis.mdb and CCDFGF_Data.mdb databases within the WinZip file CRA14_ANALYSISDATABASE. To utilize these databases they must be extracted from the zip file and installed on a PC running Microsoft Windows 7 or a compatible operating system. CCDFGF_Analysis.mdb contains the queries and code used in the analysis and contains links to some of the tables in CCDFGF_Data.mdb. CCDFGF_Data.mdb contains the data. The links in CCDFGF_Analysis will need to be updated to point to the correct location of CCDFGF_Data.mdb. These links can be updated using the Access menu item Linked Table Manager. The means are computed and the STEPWISE input file is generated by selecting the menu button in CCDFGF_Analysis labeled "Compute Vector Means for STEPWISE". This process also produces STEPWISE input files for the parameters. Simple regressions done to illustrate relationships between variables were computed within the software used to create the graphics, Sigma Plot. The Sigma Plot files are included in the WinZip file. A copy of CRA14_ANALYSISDATABASE.ZIP is also stored in the CMS library LIBCRA14_STPW.

Information Only

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