REQUEST FOR ADDITIONAL INFORMATION (RAI) Volume 3—Postclosure Chapter 2.2.1.3.3—Quantity and Chemistry of Water Contacting Engineered Barriers and Waste Form 1ST Set (RAIs 1 through 17) (DEPARTMENT OF ENERGY'S SAFETY ANLAYSIS REPORT Section 2.3.5—In-Drift Chemical Environment)

The information in the following RAIs is needed to verify compliance with 10 CFR Part 63.114(a)(1), (2), (3), (5), (6), and (7).

TOPIC 1: Chemistry of Water Entering Drifts

RAI #1

Provide the following additional technical bases to demonstrate that measured pore-water compositions can be used in SAR Section 2.3.5.3 to adequately represent the range of compositions in the natural system and can be used to determine the initial water compositions for the near-field chemistry model:

(a) An explanation for why the sample set used in selecting the starting waters for the near-field chemistry model is representative of the spatial and compositional ranges of waters associated with (1) fracture flow paths and (2) matrix flow paths. Discuss whether the sample set can be used throughout the entire repository.

(b) Support for the range of initial water compositions for conservative anions, such as chloride (CI) and nitrate (NO_3) that are important to corrosion.

(c) The locations for all 125 pore-water compositions available for the TSw (SNL, 2007, Section 6.6). Provide the locations in XYZ space in an electronic format that can be displayed in the DOE Geologic Framework Model. In addition, identify the 90 pore-water compositions that were considered in the screening process (described in SAR Section 2.3.5.3.2.2.1) and the 34 complete compositional analyses of pore waters that were considered in the selection of four initial pore-water inputs to the near-field chemistry model.

(d) An explanation of uncertainty and its propagation in the near-field chemistry model and performance assessment model. Also address the likely process-level causes for the bimodal distribution of the 34 sample compositions that passed the quality screening criteria (SAR, Figure 2.3.5-9).

Basis: SAR Section 2.3.5.3.3.2.1 (p. 2.3.5.57) identifies the following key assumption that is built into the near-field chemistry model: "Measured Pore-Water Compositions Adequately Represent the Actual Range of Initial Water Compositions in the Natural System."

The technical bases used to support the above assumption do not clearly identify the spatial and chemical variability in the natural system as represented by the measured pore-water compositions considered as inputs to the near-field chemistry model (e.g., the chemical similarities in bulk rock analyses do not explicitly consider anions DOE identifies as important to drip shield or waste package corrosion). The requested information is needed for NRC review of the adequacy of parameter values used in the near-field chemistry model.

RAI #2

Provide the following additional technical bases to demonstrate that the near-field chemistry (NFC) model adequately calculates a range of water compositions in the natural system:

Compare the results of the DOE NFC model with the results of the DOE thermal-hydrologicalchemical (THC) seepage model. This comparison should include, as a minimum, the following parameters as a function of time:

- Calcium
- pH
- Ionic strength
- Chloride
- Nitrate
- Chloride:nitrate ratio
- Partial pressure of carbon dioxide
- Any additional component that DOE concludes is significant to the evaluation of near-field chemistry in the performance assessment.

In addition, identify and quantify the effect of the alternative conceptual model on localized corrosion and the calculation of repository performance.

Basis: DOE uses the NFC model for TSPA to calculate the interaction between percolating pore waters and the rock matrix to represent the chemistries of fluids entering drifts (SAR Section 2.3.5.3.3.5.3). Prior to using the NFC model, the THC seepage model was used to predict the chemistry of seepage water entering the drifts (SAR Section 2.3.5.3.3.5.3). SAR Section 2.3.5.3.3.4 presents the limitations of the NFC model such as "... the model domain is implemented as plug flow, rather than modeling discrete fracture and matrix interactions." SAR Section 2.3.5.3.3.5.3 describes numerous significant differences in terms of implementation between the NFC model and its predecessor, the THC seepage model. This section also compares the two models using the feldspar dissolution rate and activation energy (E_a) for feldspar dissolution from the THC seepage model. The feldspar dissolution rate from the THC seepage model is about seven times higher than the NFC model at 23.4 °C and about 21 times the NFC model rate at 96 °C, as a result of the higher activation energy in the THC seepage model. Using the same values for the feldspar dissolution rate and the E_a for feldspar dissolution is appropriate for comparing the two model codes. However, the differences in the outputs of the two codes resulting from using their unique and individual feldspar dissolution

rates and E_a for feldspar dissolution cannot be determined from the results presented in this section (SAR Figures 2.3.5-23 and 2.3.5-24).

As presented, the NFC model and the THC seepage model appear to present alternative conceptual approaches to calculating seepage water chemistry. Although SEIS Table 5-1 acknowledges and attributes a small decrease in dose to refinements in the predicted ground water chemistry when the newer NFC model was implemented, this decrease is not discussed in SAR Section 2.3.5.3.3.4. The requested information is needed for NRC review of the technical bases presented in the SAR to support the use of the NFC model for TSPA and for the review of the potential effects of the NFC model on performance.

RAI #3

Provide the following additional technical bases for the screening process used to evaluate the integrity of the compositional analysis of pore-water samples:

(a) The rationale and technical basis for using a charge balance criterion of less than +/-10%

(b) Provide the pH value and technical basis used in screening samples for elevated pCO_2 . Also discuss the elevated pCO_2 value and technical basis used to support the value as an indicator of the degree of sample modification by microbial processes.

(c) Direct evidence to support the degree of sample modification by microbial processes. Evidence considered should include, but not be limited to, the following:

- Evidence that microbes capable of producing the organic acids identified in pore-water analyses and attributed to microbial activity exist in the pore water or core samples
- The nature and source of organic carbon adequate to generate the concentrations of organic acids identified in pore-water analyses and attributed to microbial activity
- A plausible metabolic or cometabolic pathway capable of producing the identified organic acids from the above-identified organic carbon source
- A nutrient mass balance capable of supporting the above-identified metabolic or cometabolic pathway
- Evidence that anoxic or anaerobic conditions existed in the core sample storage containers; evidence of microbial fermentation or another anoxic or anaerobic process identified as the sample modifying microbial process

Basis: SAR Section 2.3.5.3.2.2.1 identifies 34 complete compositional analyses of pore waters that were considered in the selection of four initial pore-water inputs to the near-field chemistry

model. SAR Section 2.3.4.3.2.2.1 indicates that a screening process based on a charge balance of less than +/-10% and calculated pH was used to eliminate 56 pore-water analyses from a set of 90 complete compositional analyses of pore water.

Charge balance is identified as an indicator of analysis quality and the calculated pH as a proxy for predicted elevated pCO_2 values. DOE interprets elevated pCO_2 values to indicate the degree of sample modification by microbial processes. The requested information is needed for NRC review of the technical bases and details of the implementation of the screening process.

RAI #4

Provide the mean and the standard deviation values associated with the beta distribution used to represent the ambient feldspar dissolution rate and their technical bases. Provide additional support to show that the beta distribution accounts for uncertainties with respect to timing and conditions of alteration, hydrologic properties, and mineral abundances. The response should account for uncertainties such as

- Uncertainty due to the potential contribution of vitric glass in the aluminosilicate alteration product concentration
- Uncertainty in the abundances of secondary aluminosilicate alteration products (e.g., clays and zeolites) in the rock
- Uncertainty in the temperature dependence of the feldspar dissolution rate that is described by the Arrhenius relationship
- Other uncertainties that DOE concludes would affect the calculation of feldspar dissolution rate significantly

and describe how these and other relevant uncertainties are propagated in the near-field chemistry model.

Basis: SAR Section 2.3.5.3.2.2.2 describes the uncertainty in the ambient feldspar dissolution rate and identifies this uncertainty as the source of the most uncertainty in the near-field chemistry model. DOE uses a beta distribution to represent the ambient feldspar dissolution rate. The requested information is needed for NRC review of the technical bases supporting the use of the beta distribution.

RAI #5

Explain how the uncertainty in the average E_a value is propagated in the near-field chemistry model. Also explain how uncertainty in literature-derived E_a values has been accounted for and propagated.

Provide a technical basis for applying an E_a value calculated from laboratory-derived feldspar dissolution rate data that are an order of magnitude larger than the feldspar dissolution rate calculated for the repository system. Also, discuss the uncertainty associated with applying an E_a value derived from laboratory experiments to a natural system that has potentially significant differences in geochemical conditions. Describe how uncertainty in the E_a value is propagated in the near-field chemistry model.

Basis: SAR Section 2.3.5.3.3.2.5 states that the temperature dependence of the feldspar dissolution rate is calculated using the Arrhenius relationship and a literature-derived activation energy (E_a) of 49 kJ/mol (SNL, 2007, Section 6.3.2.4.2). It appears that this E_a value was calculated by averaging six values from the open literature, which were determined by curve fitting measured feldspar dissolution rates in laboratory experiments. Consequently, these E_a values appear to be a function of the measured feldspar dissolution rates, which are typically an order of magnitude larger than the ambient feldspar dissolution rate used in the near-field chemistry model. The requested information is needed for NRC review of parameter ranges used in the near-field chemistry model.

RAI #6

The NFC model assumes chemical equilibrium between fracture and matrix waters. Fast flow-path fracture flow may cause chemical disequilibrium between fracture and matrix waters; thus the NFC model may not adequately represent the potential range of seepage water composition. Provide additional technical bases supporting the assumption that fracture and matrix waters are in chemical equilibrium. Demonstrate that seepage water compositions calculated using the NFC model adequately represent the potential range of seepage water chemistry.

Basis: In SAR Section 2.3.5, DOE used two lines of evidence to support the assumption of chemical equilibrium between matrix and fracture waters: (i) strontium and uranium isotope data and (ii) flow and transport modeling using the FEHM code. However, the isotope data only demonstrate that the fracture–matrix interactions are rapid relative to the precipitation of fracture-coating minerals, but do not demonstrate that the mineral precipitation is fast relative to downward transport through the matrix. Further, the FEHM code is a particle-tracking, finite element, heat and mass transfer code. It is not clear how the results from a particle-tracking

model that uses a diffusion coefficient can be used to demonstrate chemical equilibrium between fracture and matrix pore waters.

Further, field observations of perched and matrix pore waters from the base of the TSw (boreholes SD–7, SD–9, NRG–7a, and UZ–14) suggest that fracture and matrix waters are in chemical disequilibrium.

RAI #7

Transport in the NFC model is calculated using a plug flow approximation. Provide technical bases that demonstrate using average hydraulic properties in the NFC model appropriately captures the variability and uncertainty in seepage water compositions expected in the repository environment. Consider the impact of variable flow rates on potentially aggressive seepage water chemistry as influenced by water residence times and feldspar dissolution rates.

Basis: Transport through the NFC model domain is modeled using a plug flow approximation. This approach treats the TSw as a homogeneous 200-m- thick column with properties averaged from the four TSw repository host units (weighted average based on thickness). This approach includes combining and averaging matrix and fracture hydrologic properties and ignores the possibility of fast flow, via fractures, through the model domain. As a result, the range of residence times predicted by the model may not appropriately capture the potential range in water residence times in the repository environment. The residence time directly affects the amount of feldspar that dissolves in seepage water, which in turn affects the compositional range and corrosivity of seepage water.

RAI #8

PTn pore water compositions and interactions with the PTn lithologic unit at elevated temperatures were not included in the NFC model. Provide additional information to demonstrate that the water compositions predicted by the NFC model adequately represent the potential range of seepage water chemistry, considering lithologic unit heterogeneity, temperature, and starting water composition.

Basis: The thickness of the TSw varies by about ±50 m from the 200-m average value used in the NFC model. In areas of the repository where the TSw is less than 200-m thick, a packet of water originating 200-m above the repository would have a PTn pore water composition and would travel through some thickness of the PTn before entering the TSw unit. SAR Figures 2.3.5-22(a) and (b) demonstrate that the PTn pore water compositions can be significantly different than those of the TSw and the chemical evolution of those PTn waters could be significantly different than that of TSw waters, which were used as input to the NFC model.

RAI #9

The range, variability, and uncertainty in the output from the NFC are not provided in the SAR. Quantitatively describe the output data range, variability, and uncertainty for the following output parameters as predicted by the NFC model:

- pH
- *p*CO2
- nitrate concentration
- chloride concentration
- nitrate-to-chloride ratio
- ionic strength

Demonstrate that the NFC model output appropriately represents the uncertainty and variability in these parameters expected under ambient and thermally perturbed repository conditions. Consider comparisons with site characterization data; process-level modeling results, and/or field test data.

Basis: SAR Section 2.3.5.3.2 describes parametric uncertainty and the propagation of that uncertainty into the NFC model. However, no model output is provided or discussed. Therefore, the model results cannot be evaluated to determine whether they appropriately represent the range, variability, and uncertainty with respect to site characterization data, process-level modeling results, and Yucca Mountain field test data.

SAR Section 2.3.5.3.3.5.2 compares the NFC-model-predicted pore water evolutionary trends with observed pore water compositions. The predicted model results presented in SNL (2007, Figure 7.1-9) do not appear to capture the range and variability in observed CO_2 concentrations.

SAR Section 2.3.5.3.3.5.2 states that the measured pH varies from 6.7 to 8.3. The predicted model results presented in SNL (2007, Figure 7.1-10) do not appear to capture the stated range in pH. None of the model results presented in the SAR appear to have pH values below 7.5.

Predicted or measured ionic strength values are not presented or discussed in SAR Section 2.3.5; thus the NFC model results for ionic strength cannot be evaluated to determine whether the range, variability, and uncertainty in this parameter are adequately represented.

RAI #10

The evolutionary trends predicted by the NFC model in SAR Figure 2.3.5-22(b) appear to indicate that a majority of upper TSw water compositions will not evolve to the observed lower TSw water compositions. Explain how the NFC-model-predicted evolutionary trends in SAR

Figure 2.3.5-22(a) and (b) adequately represent the compositional trends observed in the Yucca Mountain region and the range of pore water compositions that are included in this figure.

Basis: SAR Section 2.3.5.3.3.5.2 compares the compositional trends of pore water predicted by the NFC model, as the pore water percolates through the geologic section, with observed Yucca Mountain pore water compositions. The evolutionary trends predicted by the NFC model in SAR Figure 2.3.5-22(a) show a slight decrease in calcium concentration and a large increase in potassium concentration. Some of the upper TSw water compositions appear to evolve toward compositions consistent with measured values for lower TSw waters. However, a majority of the upper TSw waters appear to evolve away from the observed lower TSw water compositions.

RAI #11

The NFC model predicts the occurrence of two alteration minerals (celadonite and phillipsite) that are not observed, or rarely observed, at Yucca Mountain. The unique thermodynamic properties of these minerals may impact the chemical equilibria with other minerals and chemical species in solution. Demonstrate that the NFC-model-predicted seepage water chemistry is not significantly affected when the model considers alteration minerals more commonly observed at Yucca Mountain.

Basis: SAR Section 2.3.5.3.3.5.2 compares the alteration minerals predicted by the NFC model with mineral assemblages observed at Yucca Mountain. The NFC model predicts the occurrence of two alteration minerals (celadonite and phillipsite) that are not observed, or rarely observed, at Yucca Mountain. SAR Equation 2.3.5-5 indicates that celadonite is an important product of a feldspar dissolution reaction that controls the potassium concentration in solution. The SAR states that while celadonite and phillipsite may not be the actual minerals that form at Yucca Mountain, the use of these minerals in the model would still result in the correct trends in the evolution of seepage water chemistry because the minerals mainly serve as sinks for elements like aluminum, potassium, and magnesium (celadonite) or aluminum, sodium, potassium, and calcium (phillipsite).

However, the use of these minerals in the NFC model, instead of those more commonly observed at Yucca Mountain, ignores the potential effect the unique thermodynamic properties of these minerals may have on the chemical equilibria with other minerals and species in solution. It is possible the NFC model would predict significantly different seepage water compositions if the model considered more commonly observed alteration minerals.

RAI #12

SAR Figure 2.3.5-24 compares a range of NFC-model-predicted CO_2 partial pressure (pCO_2) values to a single, unbounded pCO_2 value predicted by the THC seepage model. Provide

additional technical bases that the NFC model adequately represents the appropriate range, variability, and temporal evolution in pCO_2 expected for repository conditions.

Basis: In SAR Section 2.3.5.3.3.5.3, the THC seepage model is used to corroborate the NFC model by comparing results generated by the two models using many of the same input values. As part of this comparison, pCO_2 values predicted by the two models are presented as a function of time (SAR Figure 2.3.5-24). The comparison indicates that the range in pCO_2 values predicted by the NFC model does not capture the values predicted by the THC model after about 1,200 years, once the drift wall temperature drops below boiling. Only the bounding limits of the calculated pCO_2 values are presented in SAR Figure 2.3.5-24. Consequently, the adequacy of the NFC model to capture the important pCO_2 trends predicted by the THC model cannot be determined.

The pCO_2 value is a key parameter that is abstracted into the TSPA-LA and passed to the Waste Form Degradation and Mobilization submodel.

Reference:

SNL. 2007. "Engineered Barrier System: Physical and Chemical Environment." ANL–EBS–MD–000033. Rev. 06. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070907.0003.

Topic 2: Chemistry of Water in the Drifts

RAI #13

Provide additional information about propagation of uncertainty in seepage evaporation analyses performed by the In-Drift Precipitates/Salts (IDPS) model.

A) Provide additional explanation regarding how uncertainties in processes associated with the solubility/saturation point, deliquescence relative humidity, ion concentration, concentration factor, and precipitated minerals are accounted for and propagated through the model.

B) Provide an explanation for how the 7 figures included in the SAR chosen from the 102 figures presented in supporting documentation appropriately represent the range of uncertainty in figures used as model support.

C) Provide an explanation for how the model accounts for differences in trending between the literature/experimental values and the model results in the figures noted below for deliquescence relative humidity and solubility/saturation point.

D) Provide additional explanation for how the experimental data appropriately support the IDPS model given limitations in the experimental data due to such things as error margins and limited, if any, concentration factor constraints.

E) Provide additional explanation regarding how the uncertainties in the IDPS model and associated data are appropriately considered in the range of derived water chemistries used in the corrosion models.

Basis: DOE supports the use of the IDPS model based on comparison of model output to several experimental and literature data sets (SAR Section 2.3.5.5.3.3.1).

For example, individual salts were run for comparison in the IDPS model for saturation points at two temperatures and for deliquescence relative humidity. In addition, binary and ternary salt systems were calculated and results are reported to be within 20 percent of each literature value. However, although DOE asserts that the two comparisons are favorable, figures provided for the salts and salt systems show an apparently greater mismatch of data for many salts, including a lack of similar trending between data sets (e.g., SAR Figures 2.3.5.56–61 and 63). In addition, figures not included in the SAR show greater uncertainties than those included in the SAR (e.g., SNL, 2007, Figures 7-5, 7-8, 7-9, 7-10, 7-12, 7-15, 7-19, 7-20, 7-22, 7-23, 7-24, 7-26, 7-27, 7-28, 7-29, 7-30, 7-31, 7-40, 7-41, 7-46, 7-47, 7-50, 7-51, 7-52, 7-53, 7-60, 7-61, 7-65, and 7-68.) These figures show that as the complexity of the system increases, the dissimilarity between the IDPS calculated data and literature data appears to increase. However some relevant analyses appear to provide more accurate results, which includes more favorable trending between predicted and literature values (Gruszkiewicz et. al., 2007).

The SAR also provides a set of evaporation experiments using J-13 well water, concentrated synthetic J-13 water, and synthetic Topopah Spring Tuff pore water for further model support (SAR Section 2.3.5.5.3.3.1 and, Figures 2.3.5.56-58). In each of these experiments, DOE discusses problems with the predicted concentration factor based on experimental results. Ions expected to concentrate conservatively were underestimated by the model, resulting in an unexplained loss of some ions up to 47%. Furthermore, calcium and magnesium predictions "... can be off by up to two orders of magnitude..." based on the adjusted concentration factors. From the information provided in the SAR, it is not clear how apparent uncertainties in concentration factors were accounted for and propagated through the IDPS model.

References:

Gruszkiewicz, Miroslaw S., et al, "Phase Behavior of Aqueous Na-K-Mg-Ca-Cl-NO₃ Mixtures: Isopiestic Measurements and Thermodynamic Modeling." J. Solution Chem 36: 723-765. 2007.

SNL. "In-Drift Precipitates/Salts Model." ANL-EBS-MD-000045 Rev. 03, March 2007.

RAI #14

Provide additional technical basis to demonstrate that the pH uncertainty of ± 2 used in the IDPS model adequately represents the uncertainty in pH.

Basis: SAR Section 2.3.5.5.3.3.2 describes model uncertainty, including pH uncertainty. A characterization of the uncertainty in pH values is given by comparison with total inorganic carbon concentration. Uncertainty is attributed to "errors in the description of the experimental conditions, or measurement errors." These qualitative factors have not been quantified sufficiently to demonstrate that an uncertainty of \pm 2 appropriately represents the uncertainty in pH.

RAI #15

Provide a quantitative discussion of chemistry data collected (including but not limited to ion concentrations, pH, nitrate-to-chloride ratio, and changes in mineralogy as well as observations during drift entries) and an explanation for why applicable results from the drift scale heater test and passive tests (i.e., Alcove 7 and ECRB) were not used to support the IDPS model.

Basis: DOE conducted the drift scale heater tests and the Alcove 7 and ECRB passive tests to support characterization of coupled thermal-mechanical-hydrological-chemical behaviors of the in-drift environment (BSC, 2004; Green, et al., 2008). The IDPS model represents many important thermo-hydrochemical processes in the in-drift environment. However, results from these tests are not discussed in SAR Sections 2.3.5.3 or 2.3.5.5 in the context of the in-drift chemical environment, nor is the IDPS model supported by results from these or any other insitu tests.

References:

BSC 2004a. *Drift Scale THM Model.* MDL-NBS-HS-000017 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041012.0001.

Green, R.T. et al, "Examination of Thermal Refluxing in In-Situ Heater Tests." CNWRA Report, October 2008.

RAI #16

Part 1:

Provide a basis for why effects of dusts on seepage water chemistry have not been considered in the in-drift chemical environment models. Include implications of new information discussed by Peterman (2009) on seepage water chemistry. Basis: SAR Section 2.3.5.5 addresses the chemical characteristics of water in drifts. No information is provided regarding the potential effects of atmospheric or drift dusts on the IDPS model or abstraction. Dusts are expected to occur in drifts and have soluble material that may affect seepage water chemistry.

Part 2:

Evaluate new information on loss of nitrate from heated dust samples as discussed in Peterman (2009, 2008), as well as any ongoing research, with regard to Features, Events, and Processes (FEP) screening arguments for dust deliquescence (FEPs 2.1.09.28.0A and 2.1.09.28.0B), recognizing both atmospheric and tunnel dusts. Considering that the dusts for Peterman's investigation were samples taken from the drifts, discuss how the presence of organics in those samples and the associated processes affects the screening arguments for excluded FEPs "Undesirable Materials Left" (FEP 1.1.02.03.0A) and "Chemical Effects of Excavation and Construction in the Near Field" (FEP 1.1.02.00.0A.)

Basis: Screening arguments for "Dust Deliquesence" (FEPs 2.1.09.28.0A, and 0B) rely, in part, on benign nitrate-to-chloride ratios in evolved seepage water. However, Peterman (2009) shows that nitrate is lost from the soluble fractions of heated dust. This nitrate loss appears to result in nitrate-to-chloride ratios that were not considered in FEP screening. Similarly, screening arguments for FEP 1.1.02.00.0A and 1.1.02.03.0A apparently have not considered nitrate-to-chloride ratios or effects of introduced materials in Peterman (2009, 2008).

References:

Peterman, "Thermal Experiments on Atmospheric and Subsurface Dust at Yucca Mountain, Nevada," Presentation to NWTRB, Las Vegas, NV January 28, 2009.

Peterman, "Effects of Temperature on the Compositions of Soluble Salts in Dust at Yucca Mountain," Presentation to NWTRB, Las Vegas, NV January 16, 2008.

RAI #17

Quantitatively describe the intermediate-level output data ranges (pH, pCO₂, nitrate-to-chloride ratio, and ionic strength) for the IDPS model and explain why those ranges are representative of the in-drift environment when compared to uncertainty and variability in the site characterization data. Demonstrate that the values used in the TSPA compliance demonstration are consistent with the data output and uncertainty from the IDPS model. Demonstrate that variations in the pH, pCO₂, nitrate to chloride ratio, and ionic strength are appropriate to encompass uncertainty and variability in site characterization data.

Basis: SAR Section 2.3.5.5.2 addresses data inputs to the IDPS model, and SAR Section 2.3.5.5.4 discusses TSPA implementation; however, no intermediate process-level data output is discussed. Therefore, no uncertainty comparison can be made to site characterization data, and the reasonableness of the ranges of output data, such as nitate-to-chloride ratio, cannot be considered.