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May 12, 1997

Mr. Steve Zappe
Hazardous and Radioactive Materials Bureau
New Mexico Environment Department
2044-A Galisteo Street
Santa Fe, NM 87505

Reference: Correction to CAO Letter dated May 9, 1997, Responding to NMED Letter of April 29, 1997: Modeling and Parameter Selection Information

Dear Mr. Zappe:

Subsequent to the submittal of our May 9, 1997, response to the New Mexico Environment Department's request for modeling and parameter selection information, a discrepancy was discovered. The discrepancy relates to the parameters used to calculate gas generations rates. The gas generation rates in the application are higher than what is expected, as the models did not consider magnesium oxide backfill. Therefore, please find the enclosed responses to replace those submitted to you and received by your office on this date, May 12, 1997.

If you have any questions, please contact me at (505) 234-7452.

Sincerely,

Craig A. Snider
Compliance Engineer

cc w/enclosure:
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UFC 5480.00

RESPONSES TO NMED INFORMATION REQUESTS DATED April 29, 1997

Information #1

Comment:

Clarify whether gas generation rate assumptions in Appendix E1, Table E1-1, assume the presence of MgO in the repository.

Response:

There are 7 parameters in Table E1-1 that are related to gas generation rates. Each is discussed below:

Inundated Corrosion Rate for Steel with CO_2 Present (m/s) : In a correction to the parameter sheet "Inundated Corrosion Rate for Steel with CO_2" (Appendix D16, page 34N.DOC), the BRAGFLO modeling results supporting this application are based on the assumption that no MgO is placed in the repository. Assuming no MgO results in the accumulation of CO_2 gas in the repository, as MgO is specifically added to: 1) remove CO_2, 2) increase the pH of the system, and 3) decrease actinide solubility. For this application, assuming no MgO conservatively results in more cumulative gas generation. More moles of gas are generated due to the accumulation of CO_2 and the corrosion rate for steel in the presence of CO_2 (CORRWCO2 = 1.03×10^{-13} m/s) is higher than the corrosion rate without CO_2.

Inundated Corrosion Rate for Steel without CO_2 Present (m/s): As discussed above, MgO was not assumed in the gas generation model used for this application. As MgO is not assumed to remove CO_2 from the system, the inundated corrosion rate for steel without CO_2 present was not used (Appendix D16, page 33N.DOC). As stated above, the corrosion rate for CORRMCO2 is lower than the corrosion rate for steel with CO_2 present.

Humid Corrosion Rate for Steel: This parameter is set to zero based on experimental data reported in the Wang and Brush memo in appendix D11 and D16. This parameter is not affected by assumptions involving the presence of MgO backfill.

Gas Generation Rate for Microbial Degradation Under Humid Conditions (mol/kg * s): According to the Wang and Brush memo in Appendix D11 and D16, microbial degradation generates CO_2. According to the discussion in Appendix D22, Section 3.1, there does not appear to be a relationship between the pH and the rate of CO_2 generation. Therefore, this parameter is not affected by assumptions involving the presence of MgO backfill.

Gas Generation Rate for Microbial Degradation Under Inundated Conditions (mol/kg * s): According to the Wang and Brush memo in Appendix D11 and D16, microbial degradation generates CO_2. According to the discussion in appendix D22, Section 3.1, there does not appear to be a relationship between the pH and the rate of CO_2 generation. Therefore, this parameter is not affected by assumptions involving the presence of MgO backfill.

Factor β for Microbial Reaction Rates (unitless): This factor is related to the average stoichiometric factor "y" for microbial reaction by the following equation:

$$y = y_{min} + \beta(y_{max} - y_{min})$$

Stoichiometry factor "y" is defined to account for the expected proportions of gas generation products that will be generated:

CH2O = unknowns = microorganisms ➔ y gas + unknowns,

while Factor β is used to account for the consumption of microbially-generated gas through reactions with steel and steel corrosion products. Factor β is unaffected by any assumption involving the use of MgO. However, the stoichiometric factor "y" in the gas generation model is affected by assumptions involving the presence of MgO. Taking no credit for the consumption of CO_2 by MgO is conservative, as more total gas production would result. As discussed above, the gas generation model supporting this application assumes no MgO in the repository.

Anoxic Corrosion Stoichiometric Factor X (unitless): This parameter is set to eliminate the formation of magnetite as a reaction product from steel corrosion. Experimental evidence discussed by Wang and Brush (Appendix D11 and D16, p. -9-) justify this value based on expected repository temperature and oxygen conditions. This value is unaffected by assumptions involving the presence of MgO because MgO will not affect the oxygen content of the repository or the temperature.

Information #2

Comment:

Provide references to specific experimental data that support the assumption of assigning a value of 1.0 to the Anoxic Corrosion Stoichiometric Factor, as indicated [in] Appendix E1, Table E1-1.

Response:

Wang and Brush in Appendix D11 and D16 cite experimental observations from the test program as the basis for the assumption that the Anoxic Corrosion Stoichiometric Factor should be set to 1. Data which support this can be found in SAND92-7347 by Telander and Westerman (Hydrogen Generation by Metal Corrosion in Simulated Waste Isolation Pilot Plant Environments: Progress Report for the Period November 1989 through December 1992). (See also SAND96-2538.) On page ES-2of SAND92-7347, in summarizing the results, the authors state: "In low-carbon steel corrosion studies, the molar equivalency between Fe reacted and H_2 formed was satisfactory in both the ..." This conclusion is the basis for Wang and Brush's statement that H_2 was not observed in excess of the Fe reacted, thereby arguing against a value for "x" in Equation 11 (on page -6- of Wang and Brush) other than 1.

Information #3

Comment:

DOE/WID asserts in Appendix E1, page E1-1, lines 28 - 30, that they are ". . . seeking to demonstrate, to a reasonable degree of certainty, that there will be no migration of hazardous waste or hazardous constituents via groundwater for as long as the waste remains hazardous." In Appendix E1, Tables E1-3 and E1-4, note "a" indicates that median values for Salado formation halite and anhydrite parameters were used in modeling calculations, based upon the data and parameter distributions contained in Appendix D16, Section D16-6. However, 20 NMAC 4.1, Section V, §264.90(b) (4) states that, "In order to provide an adequate margin of safety in the prediction of potential migration of liquid, the owner or operator must base any predictions made under this paragraph on assumptions that maximize the rate of liquid migration. It is not clear how the use of median values maximize the rate of liquid migration, and it appears that worst-case assumptions have not been modeled in a single realization. Section 8.1.1 of the CCA identifies Salado anhydrite interbeds as a potential pathway to the facility boundary, and demonstrates that nine out of 300 realizations indicate releases are possible. Justify how the use of median values maximize the rate of liquid migration in modeling calculations. Alternately, submit modeling results based on worst-case assumptions that maximize the rate of liquid migration.

Response:

While it is true the standards at 20 NMAC 4.1 Subpart V §264.90(b)(4) states that a demonstration of no-migration requires assumptions that tend to maximize the rate of flow, this does not necessarily require the use of worst case values for permeability or any other hydrologic parameter. This is particularly true for the case at the WIPP, where flow during the post-closure period depends entirely on the pressure created in the disposal room and the quantity of brine that flows into the room. Discussion of this follows.

A range of permeabilities for the anhydrite marker beds was determined in the WIPP facility using standard in situ testing techniques as described in Appendix D16 (Parameter sheet k_ANH 2:38 PM3/11/96). In all cases, the permeability was below 10^{-17} m^2. Rocks with this permeability are classified by nearly all authors of groundwater flow texts as "impervious." Therefore, it is not reasonable to think of the marker beds as aquifers or water bearing zones in the context of the groundwater protection regulations in RCRA. Instead, the marker beds become significant only if the can become conduits through which contamination can reach potable waters in aquifers or water bearing zones. Because they have the highest permeabilities of all the members of the Salado in the vicinity of the repository, they become the most likely pathways for migration under certain conditions. In order for liquids to flow through these beds, one must either model over extremely long time frames (for example 10,000 years of opposed to the 30 year post-closure period), or increase the driving forces (pressure) to high levels. In the case of the nine CCA simulations referred to in the comment, both high pressures and long time frames (as well as high radionuclide solubilities) are necessary for contaminants to migrate to the boundary. In these simulations, while all had permeabilities greater than the mean, only one was actually near the high end of the permeability range. In all cases, however, the gas pressures were high, including, in some instances, enough gas to locally fracture the anhydrites.

The statements in Appendix E1, Page E1-33 beginning at line 28 indicate that conservative assumptions were used to purposely maximize the potential for gas generation in the simulation. This was to assure that the potential for flow in the marker beds was maximized as required by 20 NMAC 4.1 Subpart V §264.90(b)(4). These assumptions, as discussed in appendix E1, include:

- The entire inventory of ferrous metal, cellulosics, plastics, and rubber are available to generate gas.

- No credit taken for the 50 percent probability that biodegradation might not occur as discussed in the Wang and Brush memo in appendix D11 and D16.

- Anoxic conditions exist from the outset even though oxic conditions and the associated lower gas generation rates are likely until the shafts are sealed.

- No credit taken for de-watering of the disturbed rock zone (DRZ) during operation of the facility even though this is observed to occur throughout operations.

- The repository is assumed to be filled and sealed instantaneously so that gas pressurization begins during the period in the model when brine flow into the disposal room is greatest. In reality, much of this gas will leak into the ventilation system prior to sealing the shafts as indicated by the discussion of the panel closure design in Chapter I.

- The DRZ permeability remains high throughout the simulation even though it is subject to the compaction forces generated by salt creep. This assures a conduit to drain brine from other portion of the Salado into the disposal rooms.

An additional conservatism not pointed out in the text is the effect of dip. The waste region is modeled as being down dip from the rest of the repository. This tends to maximize the brine saturation in the waste over that in the rest of the repository.

The net effect of these conservative assumptions is to assure that there is plenty of brine for gas generation to proceed at maximum rates during the initial years following sealing the repository. The observation that repository saturation in Figure E1-16 continues to increase for the first 50 years after closure indicates that brine is flowing into the repository faster than is can be consumed by gas generating processes. This means that gas generation processes are proceeding at the highest rates possible, thereby maximizing the potential for groundwater movement into and through the marker beds.

In summary, modeling the permeability of the marker beds affects the inflow of brine and consequent gas generation in the repository, and causes the increase in pressure in the repository and subsequent flow outward. The median values used for the marker bed permeability, when combined with other conservative assumptions in the analysis such as the permeability of the DRZ, tends to maximize the rate of flow outward.

Information #4

Comment:

Appendix E1, Figure E1-12, and text on page E1-33, lines 35-43, shows that average pressure in the waste disposal region increases with time. Comparison of the threshold values for each shaft seal component with the anticipated gas generation values indicates that approximately 50 years after shaft seal emplacement, the repository pressure will exceed the threshold pressure for seal components. Provide additional information that discusses the effects of pressure build-up in the subsurface relative to the individual and cumulative effect of shaft seals, and how this might influence contaminant migration.

Response:

According to Davies (1991) there are three physical characteristics of a rock or seal material that control the flow of gas through the rock or seal pores. These characteristics are pore fluid pressure, threshold pressure, and gas permeability. The difference between fluid pressures in the pores of the waste rooms, the seal materials, and the host rocks are the primary drivers for the movement of gas and brine between the three components of the disposal system.

The pore pressure in the repository is initially assumed to be one atmosphere (0.101 MPa). The pressure in the rock ranges from lithostatic in the far field (14.8 MPa) to near atmospheric in the near field where the disturbed rock zone is well developed and depressurization of the rock has occurred. Seal materials are assumed to have an initial pore pressure of atmospheric, however the creep closure process causes this pressure to increase rapidly, depending on assumptions about initial density and the extent of the shaft DRZ development.

The threshold pressure is defined by Davies (1991) as the pressure required to overcome capillary resistance and drive gas into the brine-filled pores of a rock. A rock that is fully saturated with brine is impervious to gas penetration until the gas pressure is high enough to overcome the capillary pressures. At that time a network of interconnected gas-filled pores is established. The sum of the existing pore pressure in the rock and the threshold pressure is the pressure that must be exceeded before gas can flow through a rock.

The final property is the intrinsic permeability. This parameter has been measured for the in situ materials and is estimated for the disposal room as creep closure occurs and for seal materials, based on known properties and on the effects of creep closure on salt consolidation. These properties are discussed in the Seal Design Report (SAND96-1326) which was provided to the NMED on October 1, 1996.

Davies has developed an empirical relationship between threshold pressure and permeability which demonstrates that higher permeabilities exhibit lower threshold pressures. The coefficients for this relationship are provided in appendix D16 as parameters "PCT_A" and "PCT_EXP".

The comparison of the pressures generated in the repository to the threshold pressures in Table E1-6 is merely an indication of whether or not sufficient pressure exists for a gas phase to exist in the porosity of the seal material and not an indication of whether or not the seal integrity is jeopardized. This latter determination must consider a number of other factors, including the pore pressure and the change in permeability that occurs with time in those seal elements that are affected by creep closure, brine saturation, and gas saturation (like the salt column).

Chapter 8 of the Final Seal Design Report discusses the migration of brine and as out of the repository through or around the shaft seals. The discussion references Appendices A, C and D of the same report for more detailed information regarding the integrity of the seals. The analysis used two repository pressures for evaluation, 7MPa and 14 MPa. Both are conservative relative to the pressures expected during the first 100 years of the post-closure period (4.9 MPa) as shown in Figure E1-16 and Table E1-2. The results are discussed in Appendix C, §C5.3. Under the most conservative assumptions used in the modeling, the most gas that invades the seals is 600 m^3. This fills the pore space of the shaft seal to an elevation of the middle concrete component (750 feet above the repository floor).

REFERENCES:

Davies, Peter B., "Evaluation for the Role of Threshold Pressure in controlling Flow of Waste-Generated Gas into Bedded Salt at the Waste Isolation Pilot Plant", SAND90-3246, Sandia National Laboratories, Albuquerque, NM, June 1991.

Sandia, 1996, "Waste Isolation Pilot Plant Shaft Sealing System Compliance Submittal Design Report", SAND96-1326, Sandia National Laboratories, Albuquerque, NM, August 1996. (Copies of this report were provided to the NMED on October 1, 1996.)

Telander, M. R., and R. E. Westerman, 1993, "Hydrogen Generation by Metal Corrosion in Simulated Waste Isolation Pilot Plant Environments: Progress Report for the Period November 1989 through December 1992", SAND92-7347, Sandia National Laboratories, Albuquerque, NM, July 1993.

Telander, M. R., and R. E. Westerman, 1993, "Hydrogen Generation by Metal Corrosion in Simulated Waste Isolation Pilot Plant", SAND96-2538, Sandia National Laboratories, Albuquerque, NM, March 1997.

Wang, Y., and Larry Brush, 1996, Memo to Martin S. Tierney on Estimates of Gas-Generation Parameters for the Long-Term WIPP Performance Assessment, Sandia National Laboratories, Albuquerque, NM, January 26, 1996.