

544 248



Sandia National Laboratories

Operated for the U.S. Department of Energy by
Sandia Corporation

Joseph F. Kanney
Carlsbad Programs Group
4100 National Parks Highway
Carlsbad, NM 88220
jfkanne@sandia.gov
(505) 234-0033

date: August 31, 2006

to: David S. Kessel (6820)

from: Joseph F. Kanney (6821)  8/31/06
Eric D. Vugrin (6821)  8/31/06

Technical Review: Laurence H. Brush (6822)

QA Review: Mario J. Chavez (6820)

subject: Updated Analysis of Characteristic Time and Length Scales for Mixing Processes in the WIPP Repository to Reflect the CRA-2004 PABC Technical Baseline and the Impact of Supercompacted Mixed Waste and Heterogeneous Waste Emplacement

1. Introduction

The Waste Isolation Pilot Plant (WIPP) was built by the U.S. Department of Energy (DOE) as a deep geologic repository for transuranic radioactive waste. MgO is emplaced in the WIPP repository along with the waste as a chemical control agent to mitigate the potential effects of significant microbial consumption of cellulose, plastics and rubber materials (CPR) in the post-closure repository environment. The MgO backfill is designed to moderate brine pH and consume microbially generated carbon dioxide (CO₂), preventing undesirable impacts upon actinide solubility and mobility.

The DOE proposed emplacement of MgO in the repository in the WIPP Compliance Certification Application (CCA, U.S. DOE 1996). The DOE originally proposed placing one 4000-lb MgO sack (MgO super-sack) on top of each waste stack, as well as 25-lb MgO sacks (MgO mini-sacks) between waste stacks and on the floor surrounding waste stacks. The amount of MgO emplaced with this scheme was significantly greater than the estimated amount needed to consume all CO₂ generated if every mole organic carbon in the waste were converted to CO₂. The excess factor was estimated to be 1.95 (U.S. DOE 1996). In June 2000, DOE submitted a request to discontinue emplacement of MgO mini-sacks (U. S. DOE 2000). In 2001, EPA approved DOE's request to remove the MgO mini-sacks and lower the MgO excess factor to 1.67 (Marcinowski 2001).

The DOE has recently submitted a planned change request (PCR) to the U.S. Environmental Protection Agency (EPA) to reduce the MgO excess factor to 1.2 (U.S. DOE 2006). The EPA responded with a letter (Gitlin 2006) requesting, among other things, that DOE discuss how the presence of supercompacted waste, and the uncertainties in the amount of CPR disposed of at WIPP, affect the results of analyses like that done for the removal of the mini-sacks. EPA suggested that it would be

Exceptional Service in the National Interest

WIPP:1.4.1.2:PA:QA-L:543261

Information Only

prudent to revisit and update impact assessments performed to support the mini-sack elimination request.

This memorandum is designed to address EPA's request, with respect to the analysis of mixing processes. The analysis presented herein 1) provides an overview of mixing processes in the WIPP repository; 2) reviews the diffusion analysis conducted to support the MgO mini-sack elimination (Wang 2000); 3) updates the analysis to reflect changes to the technical baseline made in the 2004 Compliance Recertification Application Performance Assessment (CRA-2004) and the 2004 Compliance Recertification Application Performance Assessment Baseline Calculation (CRA-2004 PABC); and 4) discusses the impact of AMW waste and heterogeneous waste emplacement on the conclusions drawn in Wang (2000).

Wang (2000) concluded that diffusion processes alone are sufficient to mix CO₂ with WIPP brines over length scales corresponding to final room height, during times scales corresponding to maximum average brine flows. The results of the analysis presented herein indicate that this conclusion is still valid under the technical baseline established by the CRA-2004 PABC. Furthermore, the conclusions drawn in Wang (2000) were not impacted by supercompacted waste or heterogeneous waste emplacement.

Under all of the conditions considered, diffusion processes alone were found to be sufficient to mix CO₂ with WIPP brines over time and length scales characteristic of conditions in the waste panel. Since, under most flow conditions, mixing rates due to advection and dispersion should dominate over molecular diffusion, these results indicate a high level of confidence that sufficient mixing will occur throughout the regulatory period.

It should be noted that the analysis presented herein does not include gaseous diffusion of CO₂ throughout a room. Because the rate of gaseous diffusion of CO₂ is orders of magnitude faster than aqueous diffusion, gaseous diffusion of CO₂ is very rapid and will maintain uniform conditions in the areas in a room above the brine when a diffusion pathway exists. Thus, the analysis of Wang (2000) and the results presented herein can be considered conservative because gaseous diffusion is not considered.

2. Overview of Mixing Processes

CO₂ generated by microbial consumption of CPR in the waste will be transported away from the point of generation by several processes (assuming it was not consumed at the point of generation by reacting with the backfill). Bulk movement of brine in the repository will transport CO₂ by advection. Hydrodynamic dispersion (mixing caused by pore-scale velocity variations as the brine flows through the tortuous pore spaces of the waste and backfill) will cause CO₂ to spread both longitudinally and transverse to the direction of the bulk flow. In addition, CO₂ will also be transported from regions of higher CO₂ concentrations to regions of lower CO₂ via molecular diffusion as long as there are spatial concentration gradients. When there is considerable brine flow in the repository, advection and dispersion will be the dominant transport and mixing processes. In the absence of brine flow, molecular diffusion will be the dominant transport and mixing mechanism.

3. Review of Analyses Supporting Mini-Sack Elimination

Wang (2000) presented an analysis that compared a characteristic time scale for diffusion alone to mix CO₂ over a length representative of the repository height at 10,000 years to a characteristic hydraulic residence time for brine in a waste panel. The hydraulic residence time can be defined as

$$T_{hr} = \frac{V_p}{Q_b} \quad (3.1)$$

where T_{hr} is the mean hydraulic residence time (years), V_p is the waste panel pore volume (m³), and Q_b is the volumetric brine flow rate up the intrusion borehole to the Culebra (m³/year). (The hydraulic residence time is considered to be the average amount of time that a molecule of brine will remain in the panel.) Using the minimum pore volume and maximum flow rates reported for the CCA (Helton et al. 1998, p. 8-69), shown in Table 1, Wang (2000) calculated that mean hydraulic residence time would be always be greater than 450 years. Wang (2000) determined the maximum brine flow rate by selecting the vector with the maximum cumulative brine flow and dividing cumulative brine flow volume by the total time for which brine flowed up the borehole

Table 1 Minimum hydraulic time residence in waste panel (CCA)

	Wang (2000)
minimum waste panel pore volume (m ³)	2500
maximum average brine flow rate (m ³ /year)	5.5
hydraulic residence time (years)	454.5

Wang (2000) also calculated a characteristic diffusion penetration distance that would be consistent with the estimated mean hydraulic residence time. Assuming Fickian (linear) diffusion, the one-dimensional equation for solute diffusion through a homogeneous porous medium can be written as

$$\frac{\partial C}{\partial t} = D_{eff} \frac{\partial^2 C}{\partial x^2} \quad (3.2)$$

where C is the concentration of the diffusing species (M/L³), t is time, x is distance, and D_{eff} is the effective diffusion coefficient (L²/T). The effective diffusion coefficient accounts for two features: 1) diffusion occurs only through fluid-filled pores and not throughout entire volume of the porous medium; and 2) the diffusion pathway at the pore scale is a complicated and tortuous network, instead of a straight line. The effective diffusion coefficient is often modeled as

$$D_{eff} = F_f D \quad (3.3)$$

where F_f called the "formation factor" (dimensionless) and D is the free liquid diffusion coefficient (L²/T). The free liquid diffusion coefficient for CO₂ in sea water is approximately 2x10⁻⁵ cm²/sec (Li and Gregory 1974). The formation factor is a function of the porosity, tortuosity of the pores, and the constrictivity of the pores, but it is often modeled as a function of porosity alone:

$$F_f \approx \phi^2 \quad (3.4)$$

Combining equations (3.3) and (3.4), one obtains the equation used by Wang (2000) for the effective diffusion coefficient:

$$D_{eff} = \phi^2 D \quad (3.5)$$

Wang used the following expression for the characteristic diffusion penetration distance

$$L = \sqrt{D_{eff}T} \quad (3.6)$$

where T is a given time scale. In this case, the time scale of interest is the mean hydraulic residence time given above. The physical meaning of equation (3.6) derives from an analytical solution to the diffusion equation. One can obtain an analytic solution for one-dimensional diffusion into a semi-infinite slab when the concentration at one end is held at fixed value, C_0 (Cussler 1997):

$$\frac{C(x,t)}{C_0} = \text{erfc}(\xi), \quad \xi = \frac{x}{\sqrt{4Dt}} \quad (3.7)$$

where $\text{erfc}()$ is the complimentary error function (Abramowitz and Stegun 1972). For a distance $L = \sqrt{D_{eff}T}$, $\xi = 1/2$, and $C/C_0 \approx 1/2$. Thus, $L = \sqrt{D_{eff}T}$ represents the distance over which the concentration is reduced to approximately half of its initial concentration during a given time interval T.

Using the values for the post-room-closure porosity from the CCA, and a textbook value for free liquid diffusion coefficient, Wang (2000) reported a range for the effective diffusion coefficient of 6×10^{-3} m^2/year to 16×10^{-3} m^2/year and a range for the diffusion penetration length of 1.5 m to 2.6 m (see Table 2). Note that the reported lower limit of 6×10^{-3} m^2/yr should really be 5×10^{-3} m^2/yr (likely a rounding error, but it has no impact on the results). Note also that the free liquid diffusion coefficient used by Wang (2000) is one half of the published value for CO_2 diffusion in seawater. This is reasonable given that the ionic strength of WIPP brines is greater than that of seawater.

Table 2 Waste Panel Effective Diffusion Coefficient and Diffusion Penetration Length (CCA)

D (cm^2/s)	ϕ_{\min} (-)	ϕ_{\max} (-)	$(D_{eff})_{\min}$ (m^2/year)	$(D_{eff})_{\max}$ (m^2/year)	$(L_{450})_{\min}$ (m)	$(L_{450})_{\max}$ (m)
1×10^{-5}	0.4	0.7	5×10^{-3}	16×10^{-3}	1.5	2.6

Wang (2000) compared the estimated diffusion penetration distance to the height of the waste stacks after room closure. The height of the waste stack was computed as

$$h_f = \frac{h_0(1 - \phi_0)}{1 - \phi_f} \quad (3.8)$$

where h_0 , h_f , ϕ_0 , and ϕ_f are the initial room height, final room height, initial porosity, and final porosity, respectively. The initial porosity used by Wang (2000) was slightly larger than that given in the parameter database. The computed final room heights with the Wang (2000) initial porosity and the corrected porosity are shown in Table 3.

Table 3 Final room height (CCA)

h_0 (m)	ϕ_0 (-)	$(\phi_f)_{\min}$ (-)	$(\phi_f)_{\max}$ (-)	$(h_f)_{\min}$ (m)	$(h_f)_{\max}$ (m)
4	0.88	0.4	0.7	0.8	1.6
4	0.85	0.4	0.7	1.0	2.0

Wang (2000) concluded, based upon a minimum residence time of 450 years, that diffusion alone could mix CO₂ over a distance greater than the room height at closure. Correcting for the initial porosity does not change that conclusion.

Another way to look at the diffusion analysis is to compute diffusion time scales based upon final room heights and compare them to the minimum hydraulic residence times. The diffusion time scale is given by

$$T_{diff} = \frac{L^2}{D_{eff}} \quad (3.9)$$

Characteristic diffusion times computed using equation (3.9), and the corrected final room heights are shown in Table 4. One observes that the characteristic diffusion times are shorter than the characteristic hydraulic residence time.

Table 4 Characteristic time to diffuse over distance equal to final room height (CCA)

$(\phi_f)_{\min}$ (-)	$(h_f)_{\min}$ (m)	$(D_{eff})_{\min}$ (m ² /year)	T_{diff} (years)	$(\phi_f)_{\max}$ (-)	$(h_f)_{\max}$ (m)	$(D_{eff})_{\max}$ (m ² /year)	T_{diff} (years)
0.4	1.0	5.0x10 ⁻³	198	0.7	2.0	15.5x10 ⁻³	259

4. Update of Wang (2000) Analysis for CRA-2004 PABC Technical Baseline

The diffusion analysis of Wang (2000) was updated to reflect changes made to the technical baseline in the 2004 Compliance Recertification Application Performance Assessment Baseline Calculation (CRA-2004 PABC, Leigh et al. 2005), the current technical baseline. BRAGFLO simulations for the CRA-2004 PABC (Nemer and Stein 2005) provide the input data for the updated analysis.

Waste panel porosities, pore volumes, and brine flows are determined from the Replicate R1, Scenario S2 (R1S2) BRAGFLO simulations. The maximum cumulative brine flow in R1S2 is approximately 1.7x10⁵ m³, corresponding to an intrusion at 350 years (Nemer and Stein 2005, p. 140). Using 9650 years as the time interval over which the flow occurs gives a characteristic brine flow rate of approximately 18 m³/year. The minimum waste panel pore volume after room closure for R1S2 is approximately 4108 m³ (vector 97, see Attachment 1). The characteristic hydraulic residence time is then approximately 228 years (see Table 5).

Table 5 Characteristic hydraulic residence time in waste panel (CRA-2004 PABC)

$(V_p)_{\min}$ (m ³)	Q_b (m ³ /year)	T_{hr} (year)
4108	18	228

The volume-averaged porosity in the waste panel after room closure computed by BRAGFLO for RIS2 varies from approximately 0.089 (vector 97) to approximately 0.21 (vector 5). Attachment 1 describes how these values were obtained. BRAGFLO porosities can be converted to actual (SANTOS) porosities via the following relation:

$$\phi = \frac{\phi_B}{(1 + \phi_B - \phi_0)} \quad (4.1)$$

where ϕ is the actual (SANTOS) porosity, ϕ_B is the BRAGFLO porosity, and ϕ_0 is the initial porosity (which is the same for both BRAGFLO and SANTOS).

Converting the BRAGFLO porosities to actual (SANTOS) porosities, using equation (4.1), results in waste panel volume averaged porosity after room closure that vary between 0.37 and 0.58. These porosities are substituted into equations (3.5) and (3.6) to compute effective diffusion coefficients and characteristic diffusion penetration distances (see Table 6). The characteristic diffusion penetration distance ranges from 1 m to 1.58 m over time scales equal to the hydraulic residence time.

Table 6 Waste Panel Effective Diffusion Coefficient and Diffusion Penetration Length (CRA-2004 PABC)

D (cm ² /s)	ϕ_{\min} (-)	ϕ_{\max} (-)	$(D_{eff})_{\min}$ (m ² /year)	$(D_{eff})_{\max}$ (m ² /year)	L_{\min} (m)	L_{\max} (m)
1×10^{-5}	0.37	0.58	4.4×10^{-3}	10.7×10^{-3}	1.0	1.58

The minimum and maximum final room heights computed using equation (3.8) are shown in Table 7. The time to diffuse over these distances, calculated using equation (3.9), are shown in Table 8. One observes that the range of diffusion penetration distances bracket the range of final room heights, and the characteristic diffusion times are less than the hydraulic residence time.

Table 7 Final room height (CRA-2004 PABC)

h_0 (m)	ϕ_0 (-)	$(\phi_f)_{\min}$ (-)	$(\phi_f)_{\max}$ (-)	$(h_f)_{\min}$ (m)	$(h_f)_{\max}$ (m)
4	0.85	0.37	0.58	0.96	1.44

Table 8 Characteristic time to diffuse over distance equal to final room height (CRA-2004 PABC)

$(\phi_f)_{\min}$ (-)	$(h_f)_{\min}$ (m)	$(D_{eff})_{\min}$ (m ² /year)	T_{diff} (years)	$(\phi_f)_{\max}$ (-)	$(h_f)_{\max}$ (m)	$(D_{eff})_{\max}$ (m ² /year)	T_{diff} (years)
0.37	0.96	4.4×10^{-3}	209	0.58	1.44	10.7×10^{-3}	193

5. Impact of Supercompacted Waste and Heterogeneous Waste Emplacement

Hansen et al. (2004) conducted a PA, termed the AMWTP analysis, to assess the impact of supercompacted waste on repository performance. In the AMWTP analysis, certain characteristics of the supercompacted waste were explicitly modeled, so this analysis is useful for assessing the impact of supercompacted waste on the mixing processes.

Hansen et al. (2004) considered four different panel loading schemes:

1. Standard Waste (SW) Model. The standard waste model represents a room filled with a homogeneous mix of waste in 55-gallon drums, identical to the assumptions for the CCA and PAVT. The standard model represents a bounding case of high initial porosity and structurally compliant waste packages.
2. Combined Waste Model. This model assumes that stiff and structurally compliant wastes are mixed within a room. Supercompacted waste (SCW) is used for the stiff waste, and standard waste is used for the compliant waste. A mix of 2/3 supercompacted waste and 1/3 standard waste (by volume) was selected for this model.
3. Supercompacted Waste Model. This model assumes that all waste is structurally similar to supercompacted waste. This model reflects a bounding case where the initial porosity is low and the waste packages are stiff.
4. Pipe Overpack (POP) Model. This model assumes all waste is structurally similar to pipe overpacks. This model represents a bounding case where initial porosity is high and the waste packages are stiff. Results from the porosity surface calculations for 12" pipe overpacks were used for this model.

For the AMWTP analysis, 30% of the vectors used the first panel loading scheme, 30% used the second, 30% used the third scheme, and 10% used the fourth scheme. Additionally, to simulate non-uniform loading of CPR within the repository, the fraction of a single panel's volume that is filled with AMWTP waste (supercompacted and not) was varied between 0.2 and 1.

The techniques used to assess mixing processes from the previous sections were applied to each of the sets of panel loading schemes from the AMWTP analysis. Waste panel porosities, pore volumes, and brine flows are determined from the Replicate R1, Scenario S2 (R1S2) BRAGFLO simulations. As discussed in Hansen et al. (2004), the panels consisting solely of standard waste yielded a wider range of porosities and room heights after closure than those with supercompacted waste, but the panels with supercompacted waste generally had slightly higher final porosities (Table 9). Furthermore, the characteristic hydraulic residence time for the all standard waste schemes was 338 years, compared to 1220 years for mixed waste and 5180 years for all supercompacted waste (Table 10).

Table 9 Final room height (AMWTP)

Waste Forms	h_0 (m)	ϕ_0 (-)	$(\phi_f)_{\min}$ (-)	$(\phi_f)_{\max}$ (-)	$(h_f)_{\min}$ (m)	$(h_f)_{\max}$ (m)
All SW	4	0.85	0.29	0.58	0.85	1.44
1/3 SW + 2/3 SCW	4	0.85	0.58	0.64	1.44	1.69
All SCW	4	0.85	0.58	0.59	1.45	1.46
All POP	4	0.85	0.65	0.70	1.74	2.00

Table 10 Characteristic hydraulic residence time in waste panel (AMWTP)

Information Only

Waste Forms	$(V_p)_{\min}$ (m ³)	Q_b (m ³ /year)	T_{hr} (year)
All SW	2840	8.39	338
1/3 SW + 2/3 SCW	9820	8.04	1220
2/3 SW + 1/3 SCW	9830	1.90	5180
All POP	13200	15.6	846

The characteristic diffusion penetration distance ranges from the AMWTP analysis are shown in Table 11. It should be noted that for the standard waste panels, the minimum characteristic diffusion penetration distance is larger than the minimum room height, and the maximum characteristic diffusion penetration distance is larger than the maximum room height. For the panels with AMWTP waste, the minimum characteristic diffusion penetration distance is at least two and a half times larger than the maximum room height. Furthermore, the characteristic hydraulic residence times for all the loading schemes were larger than the respective characteristic times to diffuse the final room heights (Table 12), with the characteristic hydraulic residence times for panels with supercompacted waste being more than an order of magnitude larger than the diffusion times.

Table 11 Waste Panel Effective Diffusion Coefficient and Diffusion Penetration Length (AMWTP)

Waste Form	D (cm ² /s)	ϕ_{\min} (-)	ϕ_{\max} (-)	$(D_{eff})_{\min}$ (m ² /year)	$(D_{eff})_{\max}$ (m ² /year)	L_{\min} (m)	L_{\max} (m)
All SW	1×10^{-5}	0.29	0.58	2.6×10^{-3}	1.1×10^{-2}	0.94	1.90
1/3 SW + 2/3 SCW	1×10^{-5}	0.58	0.64	1.1×10^{-2}	1.3×10^{-2}	3.62	4.00
2/3 SW + 1/3 SCW	1×10^{-5}	0.58	0.59	1.1×10^{-2}	1.1×10^{-2}	7.46	7.51
All POP	1×10^{-5}	0.65	0.70	1.4×10^{-2}	1.5×10^{-2}	3.37	3.61

Table 12 Characteristic time to diffuse over distance equal to final room height (AMWTP)

Waste Form	$(\phi_f)_{\min}$ (-)	$(h_f)_{\min}$ (m)	$(D_{eff})_{\min}$ (m ² /year)	T_{diff} (years)	$(\phi_f)_{\max}$ (-)	$(h_f)_{\max}$ (m)	$(D_{eff})_{\max}$ (m ² /year)	T_{diff} (years)
All SW	0.29	0.85	2.6×10^{-3}	273	0.58	1.44	1.1×10^{-2}	194
1/3 SW + 2/3 SCW	0.58	1.44	1.1×10^{-2}	194	0.64	1.69	1.3×10^{-2}	219
2/3 SW + 1/3 SCW	0.58	1.45	1.1×10^{-2}	194	0.59	1.46	1.1×10^{-2}	195
All POP	0.65	1.74	1.4×10^{-2}	224	0.70	2.00	1.5×10^{-2}	259

To simulate non-uniform loading of CPR within the repository, a sampled parameter was introduced for the AMWTP analysis. The parameter FRACAMW represented the fraction of a single panel's volume that is filled with AMWTP waste (supercompacted and not), and this parameter was assigned a uniform distribution on [0.2,1). Larger values of FRACAMW indicate larger quantities of CPR in a single panel. For each vector in the AMWTP analysis, the characteristic time to diffuse a distance equal to the height of the panel, T_i , after closure was calculated using the following equation:

$$T_i = \frac{h_i^2}{D_{eff,i}}, i = 1 \dots 100$$

where h_i is the height of the room after closure for the i^{th} vector and $D_{eff,i}$ is the effective diffusion coefficient determined by the porosity of the i^{th} vector. Figure 1 plots the parameter FRACAMW versus

these times for each vector. A review of this figure leads to the conclusion that the diffusion times are not sensitive to the fraction of AMWTP waste in a single panel.

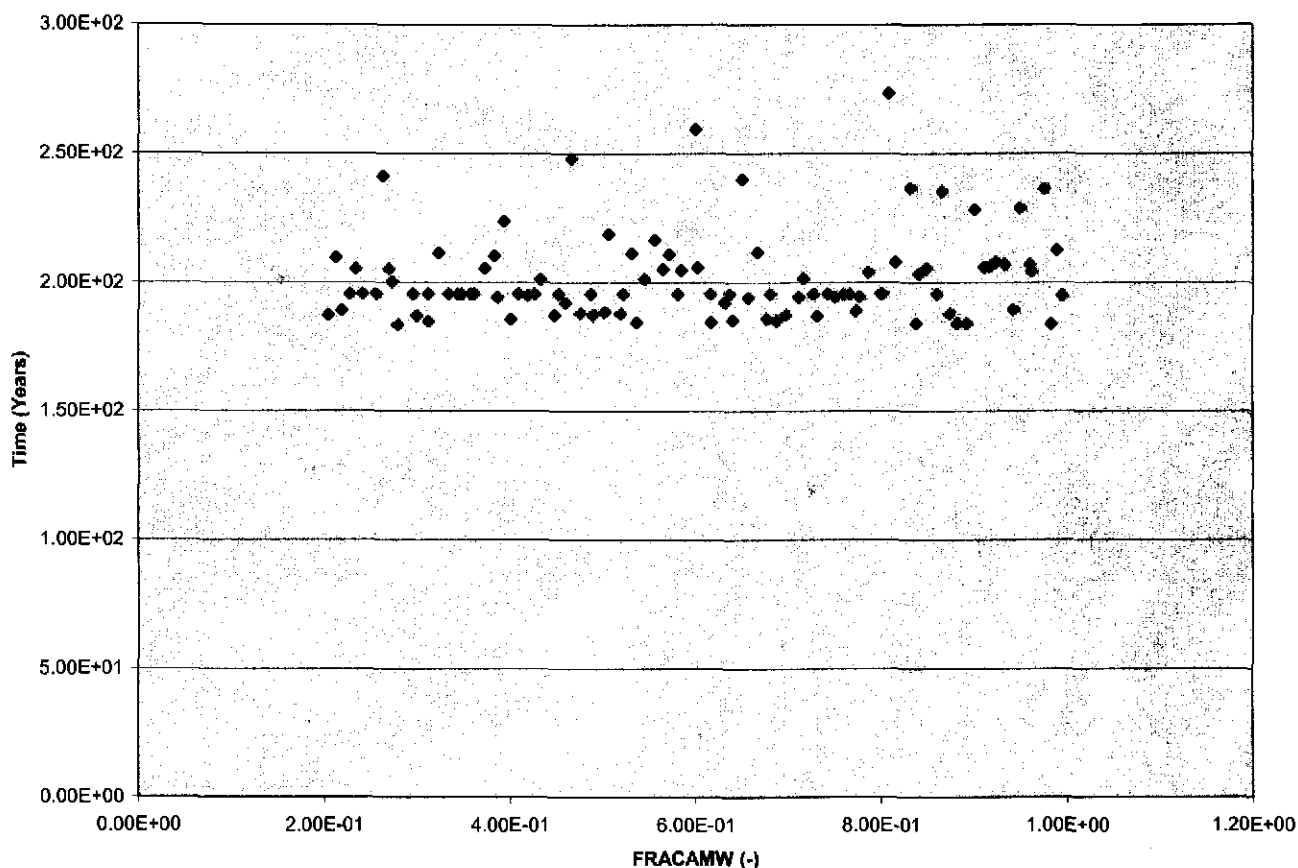


Figure 1 Scatter Plot of FRACAMW versus the Characteristic Time to Diffuse a Distance Equal to Room Height

6. Summary and Conclusions

The analysis of diffusion processes in the WIPP repository described in Wang (2000) was reviewed and a minor correction (to the initial waste panel porosity) was applied. The correction does not affect the conclusion of the analysis, that diffusion processes alone are sufficient to mix CO₂ with WIPP brines over length scales corresponding to final room height, during times scales corresponding to maximum average brine flows.

The analysis of Wang (2000) was updated for conditions that reflect the CRA-2004 PABC technical baseline. The conclusions of Wang (2000) were not changed for the new technical baseline.

The analysis of Wang (2000) was also applied in a modified form to the results of the AMWTP analysis, in order to determine the impact of supercompacted AMWTP waste and heterogeneous waste emplacement. The conclusions drawn in Wang (2000) were not impacted by supercompacted waste or heterogeneous waste emplacement.

Under all of the conditions considered, diffusion processes alone were found to be sufficient to mix CO₂ with WIPP brines over time and length scales characteristic of conditions in the waste panel. Since, under most flow conditions, mixing rates due to advection and dispersion should dominate over molecular diffusion, these results indicate a high level of confidence that sufficient mixing will occur throughout the regulatory period.

It should be noted that the analysis presented herein does not include gaseous diffusion of CO₂ throughout a room. Because the rate of gaseous diffusion of CO₂ is orders of magnitude faster than aqueous diffusion, gaseous diffusion of CO₂ is very rapid and will maintain uniform conditions in the areas in a room above the brine when a diffusion pathway exists. Thus, the analysis of Wang (2000) and the results presented herein can be considered conservative because gaseous diffusion is not considered.

References:

- Abramowitz, M., and I. Stegun. 1972. *Handbook of Mathematical Functions*. Dover, New York.
- Cussler, E. L. 1997. *Diffusion: Mass Transfer in Fluid Systems*, Second edition. Cambridge University Press, New York.
- Gitlin, B. 2006. Letter to Dave Moody, CBFO Manager. U.S. Environmental Protection Agency, Washington, DC.
- Helton, J. C., J. E. Bean, J. W. Berglund, F. J. Davis, K. Economy, J. W. Garner, J. D. Johnson, R. J. MacKinnon, J. Miller, D. G. O'Brian, J. L. Ramsey, J. D. Schreiber, A. Shinta, L. N. Smith, D. M. Stoelzel, C. Stockman, and P. Vaughn. 1998. *Uncertainty and Sensitivity Analysis Results Obtained in the 1996 Performance Assessment for the Waste Isolation Pilot Plant*. Sandia Report SAND98-0365. Sandia National Laboratories, Albuquerque, NM.
- Leigh, C., J. Kanney, L. Brush, J. W. Garner, R. Kirkes, T. L. Lowry, M. Nemer, J. S. Stein, E. D. Vugrin, S. Wagner, and T. B. Kirchner. 2005. *2004 Compliance Recertification Application Performance Assessment Baseline Calculation*. ERMS 541521, Sandia National Laboratories, Carlsbad, NM.
- Li, Y. H., and S. Gregory. 1974. *Diffusion of Ions in Sea Water and in Deep Sea Sediments*. *Geochimica et Cosmochimica Acta* **38**:703-714.
- Marcinowski, F. 2001. Letter Approving Elimination of MgO Mini-sacks. ERMS 519362, U.S. Environmental Protection Agency, Washington, DC.
- Nemer, M., and J. S. Stein. 2005. *Analysis Package for BRAGFLO: 2004 Compliance Recertification Application Performance Assessment Baseline Calculation*. ERMS 540527, Sandia National Laboratories, Carlsbad, NM.
- U. S. DOE. 2000. *Proposal for Elimination of MgO Mini-sacks*. U. S. Department of Energy Carlsbad Field Office, Carlsbad, NM.
- U.S. DOE. 1996. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot*. DOE/CAO-1996-2184, U.S. Department of Energy Waste Isolation Pilot Plant, Carlsbad Area Office, Carlsbad, NM.
- U.S. DOE. 2006. *MgO Planned Change Request*. U.S. Department of Energy Carlsbad Field Office, Carlsbad, NM.
- Wang, Y. 2000. *Effectiveness of Mixing Processes in the Waste Isolation Pilot Plant Repository*. Technical Memorandum ERMS 512401, Sandia National Laboratories, Carlsbad, NM.

Attachment 1: Waste Panel Porosity and Waste Panel Pore Volume

Waste panel pore volume and the waste panel porosity are computed by the BRAGFLO code, with some additional post-processing using the ALGEBRA utility (Nemer and Stein, 2005). Computed waste panel pore volume and waste panel porosity are store in ALGEBRA variables PORVOL_W and WAS_POR, respectively. BRAGFLO output files from the 2004 CRA-PABC are stored in the Configuration Management System (CMS) libraries on the WIPP PA Alpha Cluster (replicate R1, scenario S2 output files are stored in LIBCRA1BC_BFR1S2, class CRA1BC-0). Waste panel pore volume and waste panel porosities at 10,000 years were extracted from BRAGLFO output files using the SUMMARIZE utility. Determination of the minimum waste panel pore volume and the range of waste panel porosity can be repeated using the following steps:

Step 1: Extract PABC BRAGFLO output files for R1S2 from CMS

```
$ create/dir [.alg3]
$ set default [.alg3]
$ libcralbc_bfr1s2
$ cms fetch /generation=cralbc-0 alg3*.cdb
$ set default [-]
```

Step 2: Extract the SUMMARIZE input files from CMS

```
$ libmgored
$ cms fetch /generation=diffusion sum_cralbc_waspor.inp
$ cms fetch /generation=diffusion sum_cralbc_porvolw.inp
```

Step 3: Run SUMMARIZE to extract waste panel pore volumes

```
$ summarize sum_cralbc_porvolw.inp
```

This will produce the output file SUM_CRA1BC_PORVOLW.OUT. The minimum pore volume can be obtained by inspection.

Step 4: Run SUMMARIZE to extract the waste panel porosities

```
$ summarize sum_cralbc_waspor.inp
```

This will produce the output file SUM_CRA1BC_WASPOR.OUT. The minimum and maximum porosity can be obtained by inspection.