

Sandia National Laboratories
Waste Isolation Pilot Plant

Calculation of MgO Safety Factors for the WIPP Compliance Recertification Application and for Evaluating Assumptions of Waste Homogeneity in WIPP PA

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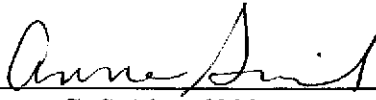
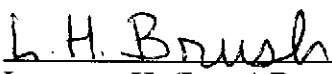

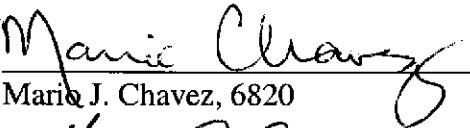
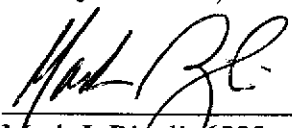
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1 ABBREVIATIONS, ACRONYMS, ETC.

Table 1 defines the abbreviations, acronyms, etc., used in this report.

Abbreviation, Acronym, Etc.	Definition
AMWTP	Advanced Mixed Waste Treatment Project
BRAGFLO	Brine and Gas Flow, a WIPP PA code
brucite	Mg(OH) ₂
C	carbon
CCA	(WIPP) Compliance Certification Application
CH	contact-handled (transuranic waste)
CPR	cellulosics, plastics, and rubbers
CO ₂	carbon dioxide
CRA	(WIPP) Compliance Recertification Application
DOE	(U.S.) Department of Energy
EPA	(U.S.) Environmental Protection Agency
ERDA-6	Energy Research and Development Administration (WIPP Well) 6, a synthetic brine representative of fluids in Castile brine reservoirs
g	gram(s)
gal	gallon(s)
GWB	Generic Weep Brine, a synthetic brine representative of intergranular Salado brines
H, H ⁺	hydrogen, hydrogen ion
hydromagnesite	Mg ₄ (CO ₃) ₃ (OH) ₂ ·3H ₂ O or Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O
IN-BN-510	the AMWTP supercompacted waste stream
INEEL	Idaho National Engineering and Environmental Laboratory
kg	kilogram(s)
lb	pound(s)
m ³	cubic meter(s)
MgO	magnesium oxide, used to refer to the WIPP engineered barrier, which includes periclase as the primary constituent and ~5-10 wt % impurities
mol	mole(s)
N	nitrogen
NO ₃ ⁻	nitrate ion, nitrate

Abbreviation, Acronym, or Initialism	Definition
O	oxygen
PA	performance assessment
periclase	pure, crystalline MgO, the primary constituent of the WIPP engineered barrier
RH	remote-handled (transuranic waste)
S	sulfur
SNL	Sandia National Laboratories
SO ₄ ²⁻	sulfate ion, sulfate
SWB(s)	standard waste box(es)
TDOP(s)	ten-drum overpack(s)
TRU	transuranic
WIPP	(U.S. DOE) Waste Isolation Pilot Plant

2 REVISION HISTORY

This analysis report has three objectives: (1) correction of the MgO safety factors for contact-handled (CH) and remote-handled (RH) transuranic (TRU) waste emplaced homogeneously in all 10 panels of the Waste Isolation Pilot Plant (WIPP); (2) correction of the safety factors calculated previously for supercompacted waste (waste stream IN-BN-510) from the Advanced Mixed Waste Treatment Project (AMWTP) at the Idaho National Engineering and Environmental Laboratory (INEEL) in a single panel for the analysis by Hansen et al. (2003), and the first calculation of additional single-panel safety factors for that analysis; (3) the first calculation of a safety factor for IN-BN-510 emplaced homogeneously in eight panels of the repository. In this report, the MgO safety factor is defined as the total quantity of MgO to be emplaced in a panel or the repository divided by the quantity of CO₂ that would be produced by complete microbial degradation of cellulose, plastics, and rubbers (CPR) in the waste or waste containers in a panel or the repository.

Correction of the MgO safety factors for a homogeneous, 10-panel repository is necessary because Lott (2003) corrected Crawford's (2003) estimates of the quantities of CPR in the CH- and RH-TRU waste and waste containers to be emplaced in the WIPP; and because Leigh and Sparks-Roybal (2003) corrected the estimates by Leigh and Crawford (2003) of the quantities of NO₃⁻ and SO₄²⁻ to be emplaced in the WIPP. The safety factors for a homogeneous, 10-panel repository reported herein replace those of

Snider (2003), which were based on the Crawford's (2003a) estimates of CPR and on Leigh and Crawford's estimates of NO_3^- and SO_4^{2-} in the inventory.

Meanwhile, Leigh (2003a, b) estimated the quantities organic ligands in a hypothetical "Panel X" for the analysis by Hansen et al. (2003). The objective of this analyses are to assess the impact of emplacing 100-gal drums of IN-BN-510 on the validity of using assumptions of waste homogeneity in WIPP PA. Leigh (2003a, b) defined two cases for this analysis: (1) a realistic case, in which the portion of the total volume of the CH TRU waste in Panel X occupied by IN-BN-510 is equal to the portion of the total volume of the CH waste in Panel 1 occupied by the largest waste stream in Panel 1, incinerator ash and process residue (waste stream RF 118.01) from the Rocky Flats Environmental Technology Site (RFETS); (2) a conservative case, in which the portion of CH waste containers in Panel X from INEEL is equal to the portion of the containers in Panel 1 from RFETS, the site that shipped the most containers to Panel 1. For both the realistic and the conservative cases, Leigh (2003a, b) assumed that the ratio of each type of CH waste container with INEEL waste in Panel X to the total quantity of INEEL CH waste containers in Panel X is equal to the ratio of the total quantity of that type of CH waste container to be shipped from INEEL to the total quantity of all the CH waste containers to be shipped from INEEL. Finally, Leigh (2003b) assumed that the total volume of CH waste in Panel X is equal to $1.685 \times 10^5 \text{ m}^3 \times 0.1044 = 17,590 \text{ m}^3$, in which $1.685 \times 10^5 \text{ m}^3$ is the total volume of CH waste to be emplaced in the WIPP and 0.1044 is the portion of the total WIPP inventory in a seven-room, PA panel (Lappin et al., 1989, Table 4-7).

Leigh (2003a, 2003b) used the assumptions described above to calculate the following for a realistic and a conservative Panel X: (1) the quantities of INEEL waste containers with IN-BN-510 and with uncompacted waste, and the quantity of containers with waste from all of the other sites; (2) the quantities of CPR and of NO_3^- and SO_4^{2-} in each type of container; (3) the total quantities of CPR and of NO_3^- and SO_4^{2-} in Panel X.

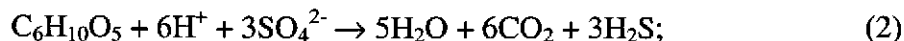
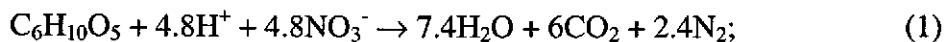
This report includes calculation of MgO safety factors for a homogeneous, 10-panel repository; a realistic Panel X, a conservative Panel X (Leigh, 2003a; 2003b), and other loadings of IN-BN-510 for the analysis by Hansen et al. (2003); and for IN-BN-510 emplaced homogeneously in eight panels.

This work was carried out under the task entitled "Chemical Conditions in the Repository" in Table 2 of Hansen et al. (2003). This report supercedes Snider (2003).

3 BACKGROUND

CPR are present in the contact handled (CH) and remote-handled (RH) TRU waste that is being or will be emplaced in the WIPP. If significant microbial activity occurs in the repository, microorganisms would degrade CPR by the following,

sequential reactions (Brush, 1990; Brush 1995; Wang and Brush, 1996; Francis et al., 1997):



Microbial degradation of CPR according to Reaction 1 (denitrification) and Reaction 2 (SO_4^{2-} reduction) would produce 1.00 mol of CO_2 per mol of organic C consumed; Reaction 3 (methanogenesis) would produce 0.500 mol of CO_2 per mol of organic C. For the CCA, Wang and Brush (1996) calculated that Reaction 3 would account for over 95% of the (possible) microbial gas generation in the WIPP. They concluded that methanogenesis would be much more important than denitrification and SO_4^{2-} reduction because the quantity of CPR greatly exceeded those of NO_3^- and SO_4^{2-} at the time of the CCA (U.S. DOE, 1996a). Based on a total quantity of 77,640 metric tons of MgO to be emplaced in the repository in supersacks and minisacks (U.S. DOE, 1996b, Chapter 3) and an effective CO_2 yield consistent with the quantities of CPR, NO_3^- , and SO_4^{2-} estimated by U.S. DOE (1996a), the MgO safety factor was 3.73 at the time of the CCA (Brush et al., 2002). The U.S. Environmental Protection Agency (EPA), however, calculated an MgO safety factor of 1.95 at the time of the CCA by assuming that microbial degradation of 1.00 mol of organic C would yield 1.00 mol of CO_2 (Brush et al., 2002).

In July 2000, the DOE proposed the elimination of the MgO minisacks to reduce the risk of injury associated with manual emplacement of the minisacks, and to further reduce worker exposure to radiation. The EPA approved this change in January 2001 (Marcinowski, 2001). Elimination of the minisacks has resulted in a 15% reduction in the total mass of MgO to be emplaced in the repository (from 77,640 to about 67,123 metric tons), and has reduced the safety factor from 3.73 to 3.23 assuming the proportions of CPR degraded by Reactions 1, 2, and 3 calculated by Brush and Wang (1996), or from 1.95 to 1.67 assuming that microbial degradation of 1.00 mol of organic C would yield 1.00 mol of CO_2 (Brush et al. 2002).

Since then, the DOE has not requested any further reductions in the MgO to be emplaced in the WIPP.

4 CALCULATIONS

All calculations were done using the Microsoft EXCEL 2000 spreadsheet program running Windows 2000. The EXCEL files are entitled "MgOsafetyfactorEPAleigh.XLS," "MgOsafetyfactorEPAleigh8panel.XLS," "MgOsafetyfactorSNLleigh.XLS," "MgOsafetyfactorSNLleigh8panel.XLS," "EPA13.5CPRpanelX.XLS," "SNL13.5CPRpanel.XLS," "EPA54CPRpanelX.XLS,"

“SNL54panelX.XLS,” and “MgOsafetyfactorSNLPAcalcs.XLS.” All of the files with “SNL” in the title assume that methanogenesis, which yields 0.50 mol of CO₂ per mol of C degraded (see Reaction 3 in Section 3, Introduction), is the dominant microbial respiratory pathway. The first four files listed above are used to calculate the MgO safety factor for a homogeneous repository with either 10 panels or 8 panels. The safety factor is calculated for a homogeneous 10-panel repository because this is the basis for “baseline” PA calculations such as those used for the CCA and the CRA; it is also calculated for a homogeneous, 8-panel repository because emplacement of waste in Panel 1 has been completed and because it is unlikely that any AMWTP waste will be shipped to WIPP prior to filling Panel 2. The next four files calculate safety factors for the realistic and the conservative Panel X defined by Leigh (2003a, 2003b) (see Section 2, Revision History, above). The final file calculates safety factors for Panel X with a range of AMWTP waste that varies from 0 to 100%.

The EXCEL files MgOsafetyfactorEPAleigh.XLS (Appendix A) and MgOsafetyfactorSNLleigh.XLS (Appendix B) each contain four sheets. The sheet tabs in each file are labeled “MgO Dissolved in Brine,” “CH CPR,” “RH CPR,” and “Safety Factor.” The files MgOsafetyfactorEPAleigh8panel.XLS (Appendix C) and MgOsafetyfactorSNLleigh8panel.XLS (Appendix D) each contain five sheets. The tabs are labeled “MgO Dissolved in Brine,” “CPR Calcs,” “CH CPR,” “RH CPR,” and “Safety Factor.” The files EPA13.5CPRpanelX.XLS (Appendix E), SNL13.5CPRpanelX.XLS (Appendix F), EPA54CPRpanelX.XLS (Appendix G), SNL54panelX.XLS (Appendix H) each contain five sheets: “MgO Dissolved in Brine,” “PA Supersack Ratio,” “CH CPR,” “RH CPR,” and “Safety Factor.” The final file, MgOsafetyfactorSNLPAcalcs (Appendix I), contains eight sheets. The sheet tabs are labeled “MgO Dissolved in Brine,” “Conservative Case,” “CH CPR,” “INEEL CPR,” “RH CPR,” “Safety Factors,” “PA Request (EPA),” and “PA Request (DOE).” Detailed descriptions of each of the four sheets present in all nine of these files (MgO Dissolved in Brine, CH CPR, RH CPR, and Safety Factor) are contained in Snider (2003). This report contains brief descriptions of each of these sheets. The first sheet in all of the files calculates the number of moles of MgO that would dissolve in GWB and ERDA-6. This is critical to the calculations because in the event of a borehole intrusion, MgO would be lost by dissolution and transport up the borehole, thus reducing the amount available to consume CO₂. Therefore, additional moles of MgO must be added to the final calculated amount in order to account for this possibility. To begin with, the initial and final concentrations of MgO were determined in both GWB and ERDA-6 from EQ3NR calculations performed by Yongliang Xiong. (These input and output files are contained in Snider, 2003.)

The second sheet in files MgOsafetyfactorEPAleigh.XLS and MgOsafetyfactorSNLleigh.XLS and the third sheet in all of the other files determines the number of moles of CO₂ that could be produced from complete microbial degradation of the CPR in CH TRU waste. Lott (2003) provided the average densities of CPR per drum of CH waste. In the file with SNL in the title, the second half of this sheet calculates the effects of including the total amounts of NO₃⁻ and SO₄²⁻ in the corrected, updated inventory (Leigh and Sparks-Roybal, 2003). The relative amounts of CPR, NO₃⁻, and

SO_4^{2-} in the inventory determine the proportions of CPR degraded by denitrification, SO_4^{2-} reduction, and methanogenesis; see Reactions 1, 2, and 3 in Section 3, Introduction. To determine the percentages of the total moles of CO_2 produced by Reactions 1, 2, and 3, the total moles of NO_3^- and SO_4^{2-} are divided by the total moles of CO_2 produced from the CPR multiplied by the stoichiometric ratio of C to NO_3^- or SO_4^{2-} , which is finally multiplied by 100. The moles left over are produced by methanogenesis. The final moles of CO_2 that could be produced from the CPR is equal to ((the molar % of cellulose degraded by denitrification) + (the molar % of cellulose degraded by sulfate reduction) + (the molar % of cellulose degraded by methanogenesis/2)) \times total moles of organic carbon (C).

The second sheet in files `MgOsafetyfactorEPAleigh8panel.XLS` and `MgOsafetyfactorSNLleigh8panel.XLS`, is entitled "CPR Calcs." This sheet takes the total CPR in kilograms for a 10-panel repository and determines the mass of CPR that will fill an 8-panel repository, assuming that Panels 1 and 2 are sealed by the time WIPP starts to emplace AMWTP waste. All INEEL waste will be distributed evenly throughout the eight remaining panels. Row 13 is the mass of CPR in INEEL waste determined by adding the 100-gal drums of supercompacted AMWTP waste + the ten-drum overpacks (TDOPs) of uncompacted AMWTP waste + the standard waste boxes (SWBs) of uncompacted AMWTP waste. Row 16 displays the mass of non-INEEL waste from all other DOE sites that will be distributed in an eight panel repository by subtracting the two seven-room panels in which waste emplacement has been completed (Panels 1 and 2) from the inventory. These numbers were calculated by taking the mass of CPR from Row 10 (55-gal drums from INEEL and all other sites) \times CPR (row 10) \times the proportion of the total WIPP inventory in two seven-room panels (2×0.1044). Row 18 is the total mass of CPR that will be distributed amongst the eight panels.

The second half of the sheet, only present in `MgOsafetyfactorSNLleigh.XLS`, repeats the same arithmetic steps just described for the CPR throughout eight panels for the masses of NO_3^- and SO_4^{2-} .

The second sheet, PA Supersack Ratio, in files `EPA13.5CPRpanelX.XLS`, `SNL13.5CPRpanelX.XLS`, `EPA54CPRpanelX.XLS`, and `SNL54CPRpanelX.XLS` determines the ratio of the number of MgO supersacks in a seven-room panel as defined for PA calculations to the number of MgO supersacks expected in a seven-room panel based on the total amount of MgO approved by the EPA when it allowed the DOE to eliminate MgO minisacks (Marcinowski, 2001). A seven-room panel as defined for PA contains $0.1044 \times$ the total CH and RH TRU waste inventory (Lappin et al., 1989, Table 4-7). This implies that there are $0.1044 \times 169,000 \text{ m}^3 = 17,591 \text{ m}^3$ of CH waste in a seven-room, PA panel (Leigh 2003b). This in turn implies that there are $17,591 \text{ m}^3 \div 0.208 \text{ m}^3/55 \text{ gal drum} = 84,574$ 55-gal drums of CH waste in a seven-room, PA panel; that there are 12,081 seven-packs of 55-gal drums in a seven-room, PA panel; and that there are 4027 MgO supersacks in a seven-room, PA panel. (One MgO supersack is emplaced atop each stack of three seven-packs of 55-gal drums, each stack of three three-packs of 100-gal drums, each stack of three SWBs, or each TDOP.) Because each MgO supersack contains 4200 lb or 1905 kg of MgO

(WTS, 2002), there are 7671 metric tons of MgO in a seven-room, PA panel. On the other hand, a total of 66,000 metric tons of MgO in the WIPP implies that there are $0.1044 \times 67,132.8 = 7008.7$ metric tons of MgO or 3679 MgO supersacks in a seven-room panel based on the mass of MgO approved by the EPA (Marcinowski, 2001). Therefore, a factor of 1.095 (Row 16 in the sheet entitled "Safety Factor") was obtained from the ratio of 4027 MgO supersacks in a seven-room, PA panel to 3679 MgO supersacks in a seven-room panel based on Marcinowski (2001). This factor of 1.095 is used to scale up the mass of MgO based on Marcinowski (2001) (Row 15 in Safety Factor) for the calculations involving the realistic and the conservative Panel X defined by Leigh (2003a, 2003b).

The third sheet in the files MgOsafetyfactorEPAl Leigh.XLS and MgOsafetyfactorSNLLeigh.XLS, and the fourth sheet in all of the other files (except MgOsafetyfactorSNLPAlcalcs.XLS), lists the CPR inventory for RH waste and the total moles of CO₂ that could be produced from possible microbial degradation of this CPR.

The final sheet in all of the files (except file MgOsafetyfactorSNLPAlcalcs.XLS) shows how the safety factors were determined. A different safety factor was determined for each file based on the previously stated assumptions of CO₂ yields and the definition of Panel X (realistic or conservative). The safety factors were determined by adding the total possible moles of CO₂ that could be produced by complete degradation of CPR to the total moles of MgO dissolved in the ERDA-6 brine. The final result is divided into the total moles of MgO in Panel X or the WIPP.

The final file, MgOsafetyfactorSNLPAlcalcs.XLS, fulfills a request by the PA personnel for information to be used in the computer code Brine and Gas Flow (BRAGFLO). This file contains sheets that carry out calculations that have not been described previously. However, the file does contain the four sheets that are present in all the previously mentioned EXCEL files.

The second sheet in the file, labeled Conservative Case, contains two parts. The top half of the sheet contains the total mass of CPR in Panel X, the mass of CPR per container type, and the total mass of CPR present in Panel X for each container. The total 55-gal mass represents all the CH waste from all the waste generation and storage sites, excluding INEEL. The three other waste containers (100-gal, SWBs and TDOPs) added together give the total mass of waste in Panel X from INEEL. To the right of the CPR table are additional columns containing such information as the emplaced waste volume, the percentage of each type of container, and the percentage by volume that each type of waste occupies in Panel X. The number of containers and container volumes are from Leigh (2003a, 2003b). The numbers of containers are multiplied by the mass of CPR per container to get the total mass of CPR in Panel X. The waste volume was determined by taking the number of containers and multiplying by individual container volumes. The lower half of the spreadsheet lists the masses of NO₃⁻ and SO₄²⁻ in Panel X, as total, per container, and total for the containers in the repository. Again, the total masses in 55-gal drums represent all the NO₃⁻ and SO₄²⁻ present in the CH waste

excluding INEEL. The masses in 100-gal drums, SWBs, and TDOPS were added together to obtain the total masses of NO_3^- and SO_4^{2-} present in INEEL waste.

The fourth sheet, INEEL CPR, is calculated in the same fashion as the third (CH CPR) and fifth (RH CPR) sheets, which have been previously described. The masses of CPR used in the fourth sheet come from masses calculated from the sheet Conservative Case.

The sixth and seventh sheets, PA Request (EPA) and PA Request (DOE) contain a table of data to be used in BRAGFLO. The table is based on 1.00 m^3 of waste starting from the conservative case where 54% of containers in panel X contain INEEL supercompacted and nondebris waste. As the non-INEEL waste is removed from 1.00 m^3 the INEEL waste is emplaced in the resulting void volume. The safety factor is obtained for each waste:INEEL waste ratio. The table is presented in the following manner:

1. Columns A and C are volumetric proportions of both CH waste from all sites except INEEL and waste from INEEL. Each row adds up to 1.00 m^3 .
2. Columns B and D are scaled percent of the volume for each waste group starting from the conservative case.
3. Columns E and F are the number of moles of non-INEEL CH waste or INEEL waste present in each volume. The initial moles of CPR in non-INEEL CH waste, starting from the conservative case, was obtained from the sheet CH CPR (E37), whereas the initial moles of INEEL waste were obtained from sheet INEEL CPR (E40). The moles in both cases were scaled up or down accordingly.
4. For sheet PA Request (DOE), columns G through K and columns L through P are calculations that determine the percent degradation from the three possible pathways, denitrification, SO_4^{2-} reduction, and methanogenesis, and are scaled accordingly for the changes in volume for each waste type. Column G is the original moles of CO_2 produced for non-INEEL waste before correction for denitrification, SO_4^{2-} reduction, and methanogenesis. The original moles are found in sheet CH CPR, Column I, Row 9. The moles are multiplied by Column B (the scaled vol %). Column H, fraction % of denitrification is computed by: (moles of nitrate/original moles of CO_2 produced from CPR) \times the stoichiometric ratio (6/4.8) \times 100. Column I, fraction % of sulfate reduction is calculated as above, except the stoichiometric ratio is 2. The fraction % or methanogenesis (column J) subtracts the total of column H and I from 100. Column K calculates the total moles of CO_2 produced from CH waste accounting for denitrification, sulfate reduction and methanogenesis by: (fraction % denitrification/100) + (fraction % SO_4^{2-} reduction/100) + (fraction % methanogenesis/100/2) \times column G. Methanogenesis is divided by 2 because 1.00 mole of C produces 0.50 mole CO_2 . Columns L through P are calculated in the same way except the moles of CO_2 are from INEEL waste only.
5. Column Q from sheet PA Request (DOE) and column G from sheet PA Request (EPA) displays how many moles of MgO will be emplaced in one panel of the repository (the current design-basis quantity of MgO).
6. Column R from PA Request (DOE) and column H from PA Request (EPA) is the total moles of CO_2 that will be produced from all the CPR in Panel X. The column is an addition of columns K and P and the amount of dissolved MgO that could be lost up a borehole and the amount of CO_2 produced from RH waste.

7. The safety factors are listed in Column S in the PA Request (DOE) sheet and Column I in the PA Request (EPA) sheet.

5 RESULTS

The corrected, updated quantities of CPR, NO_3^- , and SO_4^{2-} used in these current calculations are listed in Table 1 below.

Table 1. Densities and Masses of CPR, Nitrate, and Sulfate.

	Cellulosics	Plastics	Rubbers	Plastic liner	Nitrates	Sulfates	Waste Volume
Homogeneous							
	<u>kg/m³</u>	<u>kg/m³</u>	<u>kg/m³</u>	<u>kg/m³</u>	<u>kg</u>	<u>kg</u>	<u>m³</u>
CH	5.80E+01	1.40E+01	4.20E+01	1.60E+01	2.50E+06	4.21E+05	1.69E+05
RH	4.50E+00	4.90E+00	3.10E+00	1.40E+00	0.00E+00	0.00E+00	7.08E+03
Panel X							
	<u>kg</u>	<u>kg</u>	<u>kg</u>	<u>kg</u>	<u>kg</u>	<u>kg</u>	<u>m³</u>
Realistic	9.34E+05	6.38E+05	2.23E+05	2.86E+05	2.31E+05	1.20E+04	1.76E+04
Conservative	1.56E+06	1.08E+06	4.02E+05	2.32E+05	1.56E+06	1.08E+06	1.76E+04
RH	4.50E+00	4.90E+00	3.10E+00	1.40E+00	0.00E+00	0.00E+00	7.39E+02

The MgO safety factors and other results obtained from these calculations are described briefly below. In the following discussion, “DOE safety factor” refers to an MgO safety factor calculated using the quantity of CO_2 that would be produced by complete microbial degradation of CPR in a panel or the repository by denitrification, SO_4^{2-} reduction, and methanogenesis (see Reactions 1, 2, and 3 in Section 3, Background) in proportion to the molar quantities of NO_3^- , SO_4^{2-} , and $\text{CPR} + (\text{NO}_3^- + \text{SO}_4^{2-})$, respectively in a panel or the repository; and “EPA safety factor” refers to a safety factor calculated by assuming a quantity of CO_2 that would be produced by complete degradation of the CPR by denitrification and/or SO_4^{2-} reduction.

For a homogeneous, 10-panel repository, 4.72% of the total mass of CPR would be degraded by denitrification, 0.82% by SO_4^{2-} reduction, and 94.46% by methanogenesis; and the DOE safety factor is 2.45. The EPA safety factor is 1.30.

For a realistic Panel X, 4.48% of the total mass of CPR would be degraded by denitrification, 0.66% by SO_4^{2-} reduction, and 94.86% by methanogenesis; and the DOE safety factor is 2.66. The EPA safety factor is 1.39. These safety factors are higher than those calculated for a homogeneous, 10-panel repository (see above) because the amount of MgO assumed to be emplaced in Panel X in this report, 7670 metric tons, is 10.9%

higher than the amount consistent with a 10-panel repository that contains 74,000 short tons of MgO, the amount cited by the EPA when it approved the removal of MgO minisacks (Marcinowski, 20001, MgO Mini-sack Review, Table 1).

For a conservative Panel X, 3.00% of the total mass of CPR would be degraded by denitrification, 0.16% by SO_2^{2-} reduction, and 96.84% by methanogenesis; and the DOE safety factor is 2.02. The EPA safety factor is 1.05.

For an eight-panel, homogeneous repository, 4.87% of the total mass of CPR would be degraded by denitrification, 0.90% by SO_2^{2-} reduction, and 94.23% by methanogenesis; and the DOE safety factor is 2.14. The EPA safety factor is 1.14.

6 REFERENCES

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APPENDIX A: MgOsafetyfactorEPAIleigh.XLS

MgO Dissolved in brine

	A	B	C	D	E	F	G	H
1								
2								
3								
4								
5	GWB	Moles of MgO dissolved in brines						
6								
7		Initial and final concs by		EQ3	done by	Yongliang Xiong		
8	Concentration of Mg in brine							
9						Molality to molarity ratio factor		1.146
10		Initial Conc	Final Conc in equil	Final Conc				
11		Mol/L	with MgO, mol/Kg	mol/L				
12	Mg	1.000	7.8996E-01	6.89E-01				
13								
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs						
15								
16						Molality to molarity ratio factor		1.137
17	ERDA-6	Calculated by EQ3						
18								
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO		
20		Mol/L	with MgO, mol/Kg	mol/L	m3 *	dissolved		
21	Mg	0.019	1.0044E-01	8.83E-02	1.46E+05	1.01E+07		
22								
23								
24								
25								
26								
27								
28								
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in Bragflow							

CH CPT2

	A	B	C	D	E	F	G	H	I	J	K
1	Letter 2003, Waste Material Parameter Disposal Inventory					Average drum of CH waste					
2											
3		Formula	Avg Density	Cellulosic	volume	weight	Total moles	Total moles			
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	of C	of CO2			
5	Cellulosics	162	58	58							
6	Rubber	162	14	14							
7	Plastics	162	42	71.4							
8	Container plastic	162	16	27.2							
9	Total Cellulosics			170.6	1.7E+05	2.9E+07	1.1E+09	1.1E+09			
10											
11											
12											
13	Wang and Brush (1996)										
14											
15	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence:										Q=1.7P+R
16											
17	162 g/mol was used for all cellulosics										
18											
19	Assume 1 mole of C = 1 mole to CO2										
20											
21	PA parameter data base										
22	Total volume of CH waste		1.69E+05								

RH CPR

	A	B	C	D	E	F	G	H	I	J	K	
1	<u>Letter 2003, Waste Material Parameter Disposal Inventory</u>				Average drum of CH waste							
2												
3		Formula	Avg Density	Cellulosic	volume	weight	Total moles	Total moles				
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	of C	of CO2				
5	Cellulosics	162	4.5	4.5								
6	Rubber	162	3.1	3.1								
7	Plastics	162	4.9	8.33								
8	Plastic liners	162	1.4	2.38								
9	Total Cellulosics			18.31	7.1E+03	1.3E+05	4.8E+06	4.8E+06				
10												
11												
12	<u>Wang and Brush (1996)</u>											
13												
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence:										Q=1.7P+R	
15												
16	162 g/mol was used for all cellulosics											
17												
18	Assume 1 mole of C = 1 mole of CO2											
19												
20	<u>PA parameter data base</u>											
21	Total volume of RH waste		7.08E+03									

Information Only

Safety Factor

	A	B	C	D	E	F	G	H	I	J
1										
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.									
3										
4										
5			Volume							
6		Moles	m3							
7	Mg dissolved	1.01E+07								
8	Max CO2 generated	1.07E+09								
9	Max CO2 (RH)	4.80E+06								
10	Total MgO required	1.08E+09								
11										
12							Total Metric Tons of MgO is from Marcinowski, 2001			
13	Total MgO currently being emplaced in WIPP						7.40E+04	short tons		
14							9.07E-01	conversion factor		
15		2001 MgO minisack elimination report.					6.71E+04	metric tons		
16										
17										
18		Tons	kg	g	moles	85% react				
19		6.71E+04	67132800	6.71E+10	1.67E+09	1.41E+09				
20										
21										
22										
23	Safety Factor with new inventory data assuming one mole of C produces one mole CO2									
24										
25		Safety Factor		1.30E+00						

APPENDIX B: MgOsafetyfactorSNLeigh.XLS

MgO Dissolved in Brine

	A	B	C	D	E	F	G	H	I
1									
2									
3									
4									
5	GWB	Moles of MgO dissolved in brines							
6									
7		Initial and final concs by		EQ3	done by	Yongliang Xiong			
8	Concentration of Mg in brine								
9									
10		Initial Conc	Final Conc in equil	Final Conc					
11		Mol/L	with MgO, mol/Kg	mol/L		Molality to molarity ratio factor			1.146
12	Mg	1.000	7.8996E-01	0.6893194					
13									
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs							
15									
16									
17	Castile	Calculated by EQ3				Molality to molarity ratio factor			1.137
18									
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO			
20		Mol/L	with MgO, mol/Kg	mol/L	m3	dissolved			
21	Mg	0.019	1.0044E-01	8.8338E-02	1.46E+05	1.01E+07			
22									
23									
24									
25									
26									
27									
28									
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in BRAGFLO								

CH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Letter 2003, Waste Material Parameter Disposal Inventory					Average drum of CH waste					
2											
3		Formula	Avg Density	Cellulosic	volume	weight	Total moles	Total moles			
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	of C	of CO2			
5	Cellulosics	162	58	58							
6	Rubber	162	14	14							
7	Plastics	162	42	71.4							
8	Container plastic	162	16	27.2							
9	Total Cellulosics			170.6	1.7E+05	2.9E+07	1.1E+09	1.1E+09			
10											
11											
12	Wang and Brush (1996)										
13											
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
15											
16	162 g/mol was used for all cellulose										
17											
18	PA parameter data base										
19	Total volume of CH waste			1.69E+05							
20											
21											
22											
23	Moles of Nitrate and Sulfate Initially Present in the Waste					*from "Final Estimate of Oxyanion Mass in TRU Waste for Disposal in WIPP for the Compliance Recertification".					
24											
25		kg*	g	fw	moles						
26	Nitrate (NO3)	2.50E+06	2.50E+09	62.01	4.03E+07						
27	Sulfate (SO4)	4.21E+05	4.21E+08	96.06	4.38E+06						
28											
29											
30	Molar fraction of cellulose biodegraded via denitrification						4.72				
31											
32	Molar fraction of cellulose biodegraded via sulfate reduction						0.82				
33											
34	Molar fraction of cellulose from methanogenesis						94.46				
35											
36					moles						
37	Total CO2 production for the repository					5.63E+08					

RH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Letter 2003. Waste Material Parameter Disposal Inventory					Average drum of RH waste					
2											
3		Formula	Avg Density	Cellulosic	volume	weight	Total moles	Total moles			
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	of C	of CO2			
5	Cellulosics	162	4.5	4.5							
6	Rubber	162	3.1	3.1							
7	Plastics	162	4.9	8.33							
8	Plastic liners	162	1.4	2.38							
9	Total Cellulosics			18.31	7.1E+03	1.3E+05	4.8E+06	2.4E+06			
10											
11	Wang and Brush (1996)										
12											
13	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence:										Q=1.7P+R
14											
15	162 g/mol was used for all cellulosics										
16											
17	PA parameter data base										
18	Total volume of RH waste		7.08E+03								

SAFETY FACTOR

	A	B	C	D	E	F	G	H	I	J	K	
1												
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.											
3												
4			Volume									
5		Moles	m3									
6	Mg dissolved	1.01E+07										
7	Max CO2 generated	5.63E+08										
8	Max CO2 (RH)	2.40E+06										
9	Total MgO required	5.76E+08	1.45E+04									
10							Total Metric Tons of MgO is from Marcinowski, 2001					
11							7.40E+04	short tons				
12							9.07E-01	conversion factor				
13	Total MgO currently being emplaced in WIPP							6.71E+04	metric tons			
14												
15	Tons	Kg	g	moles	85% react							
16	6.71E+04	67132800	6.71E+10	1.67E+09	1.41E+09							
17												
18												
19												
20	Safety Factor with new inventory data assuming one mole of C produces one mole CO2											
21												
22	Safety Factor		2.45E+00									

APPENDIX C: MgOsafetyfactorEPAleigh8panel.XLS

MgO Dissolved in Brine

	A	B	C	D	E	F	G	H
1								
2								
3								
4								
5	GWB	Moles of MgO dissolved in brines						
6								
7		Initial and final concs by		EQ3	done by	Yongliang Xiong		
8	Concentration of Mg in brine							
9						Molality to molarity ratio factor		1.146
10		Initial Conc	Final Conc in equil	Final Conc				
11		Mol/L	with MgO, mol/Kg	mol/L				
12	Mg	1.000	7.8996E-01	6.89E-01				
13								
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs						
15								
16						Molality to molarity ratio factor		1.137
17	ERDA-6	Calculated by EQ3						
18								
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO		
20		Mol/L	with MgO, mol/Kg	mol/L	m3*	dissolved		
21	Mg	0.019	1.0044E-01	8.83E-02	1.46E+05	1.01E+07		
22								
23								
24								
25								
26								
27								
28								
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000- yrs) in Bragflow							

02

CPR Calcs

	A	B	C	D	E	F	G	H
1								
2	From Leigh 2003 "Estimate of Cellulosics, Plastic, and Rubber in a Singel Panel in the WIPP Repository in Support of AP-107"							
3								
4								
5		Vol (m3)	Cell (kg)	Plastic (kg)	Rubber (kg)	Plastic liner (kg)		
6	Whole repository	1.69E+05	9.77E+06	7.08E+06	2.36E+06	2.70E+06		
7	100 gal supercompacted INEEL	1.99E+04	6.02E+06	4.07E+06	1.59E+06	0.00E+00		
8	TDOPS non-debris INEEL	3.42E+04	9.18E+04	1.21E+05	3.14E+02	6.53E+05		
9	SWBs from INEEL	6.75E+03	1.85E+04	2.40E+04	6.83E+01	1.08E+05		
10	55-gal from INEEL and all sites	1.08E+05	3.64E+06	2.87E+06	7.70E+05	1.94E+06		
11								
12								
13	1) INEEL; all distributed over 8 panels	1.34E+05	6.13E+06	4.22E+06	1.59E+06	7.61E+05		
14								
15	55-gal from INEEL and all sites		3.64E+06	2.87E+06	7.70E+05	1.94E+06		
16	2) non-INEEL; for 8 panel	1.34E+05	2.88E+06	2.27E+06	6.09E+05	1.53E+06		
17								
18	Total for an eight panel repository	1.34E+05	9.01E+06	6.49E+06	2.20E+06	2.30E+06		

CH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Letter 2003, Waste Material Parameter Disposal Inventory					Average drum of CH waste					
2											
3		Formula	Avg Density	Cellulosic	volume	weight	equivalent	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	kg	of C	of CO2		
5	Cellulosics	162	6.72E+01	67.2		9.01E+06					
6	Rubber	162	1.64E+01	16.4		2.20E+06					
7	Plastics	162	4.84E+01	82.3		6.49E+06					
8	Container plastic	162	1.71E+01	29.1		2.30E+06					
9	Total Cellulosics			195	1.3E+05	2.00E+07	2.6E+07	9.7E+08	9.7E+08		
10											
11											
12											
13	Wang and Brush (1996)										
14											
15	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
16											
17	162 g/mol was used for all cellulose										
18											
19	Assume 1 mole of C = 1 mole of CO2										
20											
21	PA parameter data base										
22	Total volume of CH waste		1.69E+05								

RH CIR

	A	B	C	D	E	F	G	H	I	J	K	
1	Letter 2003, Waste Material Parameter Disposal Inventory				Average drum of RH waste							
2												
3		Formula	Avg Density	Cellulosic	volume	weight	Total moles	Total moles				
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	of C	of CO2				
5	Cellulosics	162	4.5	4.5								
6	Rubber	162	3.1	3.1								
7	Plastics	162	4.9	8.33								
8	Plastic liners	162	1.4	2.38								
9	Total Cellulosics			18.31	7.1E+03	1.3E+05	4.8E+06	4.8E+06				
10												
11												
12	Wang and Brush (1996)											
13												
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence:										Q=1.7P+R	
15												
16	162 g/mol was used for all cellulosics											
17												
18	Assume 1 mole of C = 1 mole to CO2											
19												
20	PA parameter data base											
21	Total volume of RH waste		7.08E+03									

Safety Factor

	A	B	C	D	E	F	G	H	I	J	K
1											
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.										
3											
4											
5			Volume								
6		Moles	m3								
7	Mg dissolved	8.00E+06					Volume of 8 panels	1.34E+05			
8	Max CO2 generated	9.68E+08					Volume of 10 panels	1.69E+05			
9	Max CO2 (RH)	3.80E+06					Ratio	7.93E-01			
10	Total MgO required	9.80E+08									
11											
12							Row 8 has already been corrected for 8 panels. See sheet CH CPR. Note volume is	1.34E+05			
13	Total MgO currently being emplaced in WIPP										
14											
15		2001 MgO minisack elimination report.						Total Metric Tons of MgO is from Marcinowski, 2001			
16								7.40E+04	short tons		
17											
18								9.07E-01	conversion factor		
19		Tons	kg	g	moles	85% react		6.71E+04	metric tons		
20		53115.4714	53115471	5.31E+10	1.32E+09	1.12E+09					
21											
22											
23											
24	Safety Factor with new inventory data assuming one mole of C produces one mole CO2										
25											
26		Safety Factor		1.14E+00							

APPENDIX D: MgOsafetyfactorSNLeigh8panel.XLS

MgO Dissolved in Brine

	A	B	C	D	E	F	G	H	I
1									
2									
3									
4									
5	GWB	Moles of MgO dissolved in brines							
6									
7		Initial and final concs by	EQ3	done by	Yongliang Xiong				
8	Concentration of Mg in brine								
9									
10		Initial Conc	Final Conc in equil	Final Conc					
11		Mol/L	with MgO, mol/Kg	mol/L		Molality to molarity ratio factor			1.146
12	Mg	1.000	7.8996E-01	0.6893194					
13									
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs							
15									
16									
17	Castile	Calculated by EQ3				Molality to molarity ratio factor			1.137
18									
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO			
20		Mol/L	with MgO, mol/Kg	mol/L	m3 *	dissolved			
21	Mg	0.019	1.0044E-01	8.8338E-02	1.46E+05	1.01E+07			
22									
23									
24									
25									
26									
27									
28									
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in BRAGFLO								

CPR calcs

	A	B	C	D	E	F	G	H
1								
2	From Leigh 2003 "Estimate of Cellulosics, Plastic, and Rubber in a Singel Panel in the WIPP Repository in Support of AP-107"							
3								
4								
5		Vol (m3)	Cell (kg)	Plastic (kg)	Rubber (kg)	Plastic liner (kg)		
6	Whole repository	1.69E+05	9.77E+06	7.08E+06	2.36E+06	2.70E+06		
7	100 gal supercompacted INEEL	1.99E+04	6.02E+06	4.07E+06	1.59E+06	0.00E+00		
8	TDOPS non-debris INEEL	3.42E+04	9.18E+04	1.21E+05	3.14E+02	6.53E+05		
9	SWBs from INEEL	6.75E+03	1.85E+04	2.40E+04	6.83E+01	1.08E+05		
10	55-gal from INEEL and all sites	1.08E+05	3.64E+06	2.87E+06	7.70E+05	1.94E+06		
11								
12								
13	1) INEEL; all distributed over 8 panels	1.34E+05	6.13E+06	4.22E+06	1.59E+06	7.61E+05		
14								
15	55-gal from INEEL and all sites		3.64E+06	2.87E+06	7.70E+05	1.94E+06		
16	2) non-INEEL; for 8 panel	1.34E+05	2.88E+06	2.27E+06	6.09E+05	1.53E+06		
17								
18	Total for an eight panel repository	1.34E+05	9.01E+06	6.49E+06	2.20E+06	2.30E+06		
19								
20								
21								
22	From Leigh 2003 "Estimate of Oxyanion Masses in a Single Panel in the WIPP Repository in Support of AP-107"							
23								
24		Vol	Nitrates (kg)	Sulfate (kg)				
25	Whole repository		2.50E+06	4.21E+05				
26	100 gal supercompacted INEEL		0	0				
27	TDOPS non-debris INEEL		6.51E+05	8.70E+03				
28	SWBs from INEEL		1.29E+05	2.16E+03				
29	55-gal from INEEL and all sites		1.72E+06	4.10E+05				
30								
31	1) INEEL; all distributed over 8 panels		7.80E+05	1.09E+04				
32	volume							
33								
34	2) non-INEEL; for 8 panel		1.56E+06	4.08E+05				
35								
36	Total for an eight panel repository		2.34E+06	4.19E+05				

CH CPR

	A	B	C	D	E	F	G	H	I	J	K	
1	<u>Letter 2003, Waste Material Parameter Disposal Inventory</u>					Average drum of CH waste						
2												
3		Formula	Avg Density	Cellulosic	volume	weight	Equivalent	Total moles	Total moles			
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	wt	of C	of CO2			
5	Cellulosics	162	6.72E+01	6.7E+01		9.01E+06						
6	Rubber	162	1.64E+01	1.6E+01		2.20E+06						
7	Plastics	162	4.84E+01	8.2E+01		6.49E+06						
8	Container plastic	162	1.71E+01	2.9E+01		2.30E+06						
9	Total Cellulosics			195	1.3E+05	2.00E+07	2.6E+07	9.7E+08	9.7E+08			
10												
11												
12	<u>Wang and Brush (1996)</u>											
13												
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R	
15												
16	162 g/mol was used for all cellulose											
17												
18	<u>PA parameter data base</u>											
19	Total volume of CH waste for an 8 panel repository				1.34E+05							
20												
21												
22												
23	Moles of Nitrate and Sulfate Initially Present in the Waste					*from "Final Estimate of Oxyanion Mass in TRU Waste for Disposal in WIPP for the Compliance Recertification".						
24												
25		kg*	g	fw	moles							
26	Nitrate (NO3)	2.34E+06	2.34E+09	62.01	3.77E+07							
27	Sulfate (SO4)	4.19E+05	4.19E+08	96.06	4.36E+06							
28												
29												
30	Molar fraction of cellulose biodegraded via denitrification					4.87						
31												
32	Molar fraction of cellulose biodegraded via sulfate reduction					0.90						
33												
34	Molar fraction of cellulose from methanogenesis					94.23						
35												
36					moles							
37	Total CO2 production for the repository				5.12E+08							

Information Only

RH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Letter 2003, Waste Material Parameter Disposal Inventory				Average drum of RH waste						
2											
3		Formula	Avg Density	Cellulosic	volume	weight	Total moles	Total moles			
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	of C	of CO2			
5	Cellulosics	162	4.5	4.5							
6	Rubber	162	3.1	3.1							
7	Plastics	162	4.9	8.33							
8	Plastic liners	162	1.4	2.38							
9	Total Cellulosics			18.31	7.1E+03	1.3E+05	4.8E+06	2.4E+06			
10											
11	Wang and Brush (1996)										
12											
13	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence:										Q=1.7P+R
14											
15	162 g/mol was used for all cellulosics										
16											
17	PA parameter data base										
18	Total volume of RH waste		7.08E+03								

Information Only

35

Safety Factor

	A	B	C	D	E	F	G	H	I	J	K
1											
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.										
3											
4			Volume		Row 6 and Row 8 are multiplied by a volume correction factor for a 8 panel repository. The correction factor is the ratio of the volume of 8 panels to the volume of 10 panels.						
5		Moles	m3								
6	Mg dissolved	8.00E+06									
7	Max CO2 generated	5.12E+08			Volume of 8 panels			1.34E+05			
8	Mas CO2 (RH)	1.90E+06			Volume of 10 panels			1.69E+05			
9	Total MgO required	5.22E+08	1.31E+04		Ratio			7.93E-01			
10											
11					Row 7 has already been corrected for 8 panels. See sheet CH CPR. Note						
12					volume is	1.34E+05					
13											
14											
15											
16	Total MgO currently being emplaced in WIPP										
17							Total Metric Tons of MgO is from Marcinowski, 2001				
18	Tons	Kg	g	moles	85% react		7.40E+04	short tons			
19	53115.47136	53115471.4	5.31E+10	1.32E+09	1.12E+09		9.07E-01	conversion factor			
20							6.71E+04	metric tons			
21											
22											
23	Safety Factor with new inventory data assuming one mole of C produces one mole CO2										
24											
25	Safety Factor		2.14E+00								

APPENDIX E: EPA13.5CPRpanelXupdate.XLS

MgO Dissolved in Brine

	A	B	C	D	E	F	G	H	I
1									
2									
3									
4									
5	GWB	Moles of MgO dissolved in brines							
6									
7		Initial and final concs by		EQ3	done by	Yongliang Xiong			
8	Concentration of Mg in brine								
9									
10		Initial Conc	Final Conc in equil	Final Conc					
11		Mol/L	with MgO, mol/Kg	mol/L		Molality to molarity ratio factor			1.146
12	Mg	1.000	7.8996E-01	0.6893194					
13									
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs							
15									
16									
17	Castile	Calculated by EQ3				Molality to molarity ratio factor			1.137
18									
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO			
20		Mol/L	with MgO, mol/Kg	mol/L	m3 *	dissolved			
21	Mg	0.019	1.0044E-01	8.8338E-02	1.46E+05	1.01E+07			
22									
23									
24									
25									
26									
27									
28									
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in BRAGFLO								

PA Supersack Ratio

	A	B	C	D	E	F	G	H
1								
2		PER PANEL						
3	Case 1	PA						operational
4		12082		seven packs				10908
5		3		seven packs per available space				
6		4027.333		supersacks				3636
7		16914800		Mass of MgO (lb) per panel				
8		7672425		Mass of MgO (kg) per panel				
9								
10	Case 2	operational						
11		67132800		Mass of MgO (kg) currently scheduled to be emplaced				
12		0.1044		Ratio factor for one PA panel				
13		7008664		Mass of MgO (kg) emplaced in one panel				
14		3678.919		supersacks of MgO in one PA panel				
15								
16	Ratio	1.094706						
17	# supersacks							
18								
19		supersack		4200	lb			
20		number in one panel		1905	kg			
21								
22								
23								
24								
25								Safety Factor corresponds to one supersack per stack.

CH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Average drum of CH waste for panel X assuming 13.5% of the volume is AMWTP supercompacted.										
2	Cellulosic numbers given by C. Leigh			Realistic Case							
3		Formula	Avg Density	Cellulosic	volume	weight	weight (kg)	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	cell equivalent	of C	of CO2		
5	Cellulosics	162	6.1E+01	6.06E+01		1.07E+06					
6	Rubber	162	1.5E+01	1.48E+01		2.62E+05					
7	Plastics	162	4.4E+01	7.43E+01		7.71E+05					
8	Container plastic	162	1.6E+01	2.64E+01		2.74E+05					
9	Total Cellulosics			176.18287	1.8E+04	2.4E+06	3.11E+06	1.15E+08	1.15E+08		
10											
11											
12	Wang and Brush (1996)										
13											
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
15											
16	162 g/mol was used for all cellulose										
17											
18	PA parameter data base										
19	Total volume of CH waste			1.69E+05							
20	Ratio factor for one panel			0.1044							
21	Total volume of CH waste for ONE panel			1.76E+04							

RH CPR

	A	B	C	D	E	F	G	H	I	J	K	
1	<u>Letter 2003, Waste Material Parameter Disposal Inventory</u>					Average drum of RH waste for one panel						
2												
3		Formula	Avg Density	Cellulosic	volume	weight	weight for	Total moles	Total moles			
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	one panel	of C	of CO2			
5	Cellulosics	162	6.1	6.1								
6	Rubber	162	3.6	3.6								
7	Plastics	162	7	11.9								
8	Total Cellulosics			2.25504	7.4E+02	1.7E+03	174.01573	6.4E+03	6.45E+03			
9												
10												
11	<u>Wang and Brush (1996)</u>											
12												
13	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R	
14												
15	162 g/mol was used for all cellulose											
16												
17	<u>PA parameter data base</u>											
18	Total volume of RH waste		7.08E+03									

Safety Factor

	A	B	C	D	E	F	G	H	I	J	K
1											
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.										
3											
4			Volume								
5		Moles	m3								
6	Mg dissolved	1.06E+06									
7	Max CO2 generated	1.15E+08									
8	Max CO2 (RH)	6.45E+03									
9	Total MgO required	1.16E+08	2.92E+03				Ratio factor from sheet "PA supersack ratio" row 16:			1.095	
10											
11											
12	Total MgO currently being emplaced in WIPP										
13								Total Metric Tons of MgO is from Marcinowski, 2001			
14	Tons	Kg	g	moles	85% react		7.40E+04	short tons			
15	7.67E+03	7674487.43	7.67E+09	1.90E+08	1.61E+08		9.07E-01	conversion factor			
16							6.71E+04	metric tons			
17											
18											
19	Safety Factor with new inventory data assuming one mole of C produces one mole CO2										
20											
21	Safety Factor		1.39E+00								

22

APPENDIX F: SNL13.5CPRpanelXupdate.XLS

MgO Dissolved in Brine

	A	B	C	D	E	F	G	H	I
1									
2									
3									
4									
5	GWB	Moles of MgO dissolved in brines							
6									
7		Initial and final concs by	EQ3	done by	Yongliang Xiong				
8	Concentration of Mg in brine								
9									
10		Initial Conc	Final Conc in equil	Final Conc					
11		Mol/L	with MgO, mol/Kg	mol/L		Molality to molarity ratio factor			1.146
12	Mg	1.000	7.8996E-01	0.6893194					
13									
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs							
15									
16									
17	Castile	Calculated by EQ3					Molality to molarity ratio factor		1.137
18									
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO			
20		Mol/L	with MgO, mol/Kg	mol/L	m3 *	dissolved			
21	Mg	0.019	1.0044E-01	8.8338E-02	1.46E+05	1.01E+07			
22									
23									
24									
25									
26									
27									
28									
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in BRAGFLO								

PA Supersack Ratio

	A	B	C	D	E	F	G	H
1								
2		PER PANEL						
3	Case 1	PA						operational
4		12082		seven packs				10908
5		3		seven packs per available space				
6		4027.333		supersacks				3636
7		16914800		Mass of MgO (lb) per panel				
8		7672425		Mass of MgO (kg) per panel				
9								
10	Case 2	operational						
11		67132800		Mass of MgO (kg) currently scheduled to be emplaced				
12		0.1044		Ratio factor for one PA panel				
13		7008664		Mass of MgO (kg) emplaced in one panel				
14		3678.919		supersacks of MgO in one PA panel				
15								
16	Ratio	1.094706						
17	# supersacks							
18								
19		supersack		4200	lb			
20		number in one panel		1905	kg			
21								
22								
23								
24								
25		Safety Factor corresponds to one supersack per stack.						

CH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Average drum of CH waste for panel X assuming 13.5% of the volume is AMWTP supercompacted.										
2	Cellulosic numbers given by C. Leigh			Realistic Case							
3		Formula	Avg Density	Cellulosic	volume	weight	weight (kg)	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	cell equivalent	of C	of CO2		
5	Cellulosics	162	6.1E+01	6.06E+01		1.07E+06					
6	Rubber	162	1.5E+01	1.48E+01		2.62E+05					
7	Plastics	162	4.4E+01	7.43E+01		7.71E+05					
8	Container plastic	162	1.6E+01	2.64E+01		2.74E+05					
9	Total Cellulosics			176.18287	1.8E+04	2.4E+06	3.11E+06	1.15E+08	1.15E+08		
10											
11											
12	Wang and Brush (1996)										
13											
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
15											
16	162 g/mol was used for all cellulose										
17											
18	PA parameter data base										
19	Total volume of CH waste			1.69E+05							
20	Ratio factor for one panel			0.1044							
21	Total volume of CH waste for ONE panel			1.76E+04							
22											
23	Moles of Nitrate and Sulfate Initially Present in the Waste										
24	*from "Estimate of Oxyanion in a Single Panel in the WIPP Repository in Support of AP-107 Supercedes ERMS#530988 Rev. 1"										
25		kg*	g	fw	moles						
26	Nitrate (NO3)	2.56E+05	2.56E+08	62.01	4.13E+06						
27	Sulfate (SO4)	3.63E+04	3.63E+07	96.06	3.78E+05						
28											
29											
30	Molar fraction of cellulose biodegraded via denitrification						4.48				
31											
32	Molar fraction of cellulose biodegraded via sulfate reduction						0.66				
33											
34	Molar fraction of cellulose from methanogenesis						94.86				
35											
36					moles						
37	Total CO2 production for the repository				6.05E+07						

40

RH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Letter 2003, Waste Material Parameter Disposal Inventory					Average drum of RH waste for one panel					
2											
3		Formula	Avg Density	Cellulosic	volume	weight	weight for	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	one panel	of C	of CO2		
5	Cellulosics	162	6.1	6.1							
6	Rubber	162	3.6	3.6							
7	Plastics	162	7	11.9							
8	Total Cellulosics			2.25504	7.4E+02	1.7E+03	174.01573	6.4E+03	3.2E+03		
9											
10											
11	Wang and Brush (1996)										
12											
13	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
14											
15	162 g/mol was used for all cellulose										
16											
17	PA parameter data base										
18	Total volume of RH waste		7.08E+03								

Safety Factor

	A	B	C	D	E	F	G	H	I	J	K
1											
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.										
3											
4			Volume								
5		Moles	m3								
6	Mg dissolved	1.06E+06									
7	Max CO2 generated	6.05E+07									
8	Max CO2 (RH)	3.22E+03									
9	Total MgO required	6.16E+07	1.55E+03		Ratio factor from sheet "PA supersack ratio" row 16:					1.095	
10											
11											
12	Total MgO currently being emplaced in WIPP						Total Metric Tons of MgO is from Marcinowski, 2001				
13							7.40E+04	short tons			
14	Tons	Kg	g	moles	85% react		9.07E-01	conversion factor			
15	7.67E+03	7674487.43	7.67E+09	1.90E+08	1.61E+08		6.71E+04	metric tons			
16											
17											
18											
19	Safety Factor with new inventory data assuming one mole of C produces one mole CO2										
20											
21	Safety Factor		2.62E+00								

APPENDIX G: EPA54CPRpaneIX.XLS

MgO Dissolved in Brine

	A	B	C	D	E	F	G	H	I
1									
2									
3									
4									
5	GWB	Moles of MgO dissolved in brines							
6									
7		Initial and final concs by		EQ3	done by	Yongliang Xiong			
8	Concentration of Mg in brine								
9									
10		Initial Conc	Final Conc in equil	Final Conc					
11		Mol/L	with MgO, mol/Kg	mol/L		Molality to molarity ratio factor			1.146
12	Mg	1.000	7.8996E-01	0.6893194					
13									
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs							
15									
16									
17	Castile	Calculated by EQ3				Molality to molarity ratio factor			1.137
18									
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO			
20		Mol/L	with MgO, mol/Kg	mol/L	m3 *	dissolved			
21	Mg	0.019	1.0044E-01	8.8338E-02	1.46E+05	1.01E+07			
22									
23									
24									
25									
26									
27									
28									
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in BRAGFLO								

PA Superpack Ratio

	A	B	C	D	E	F	G	H	
1									
2		PER PANEL							
3	Case 1	PA						operational	
4		12082		seven packs				10908	
5		3		seven packs per available space					
6		4027.333		supersacks				3636	
7		16914800		Mass of MgO (lb) per panel					
8		7672425		Mass of MgO (kg) per panel					
9									
10	Case 2	operational							
11		67132800		Mass of MgO (kg) currently scheduled to be emplaced					
12		0.1044		Ratio factor for one PA panel					
13		7008664		Mass of MgO (kg) emplaced in one panel					
14		3678.919		supersacks of MgO in one PA panel					
15									
16	Ratio	1.094706							
17	# supersacks								
18									
19		supersack		4200	lb				
20		number in one panel		1905	kg				
21									
22									
23									
24									
25				Safety Factor corresponds to one supersack per stack.					

CH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Average drum of CH waste for panel X assuming 54% of the containers originated from INEEL										
2	Cellulosic numbers given by C. Leigh										
3		Formula	Avg Density	Cellulosic	volume	weight	weight (kg)	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	cell equivalent	of C	of CO2		
5	Cellulosics	162	8.8E+01	8.84E+01		1.56E+06					
6	Rubber	162	2.3E+01	2.28E+01		4.02E+05					
7	Plastics	162	6.1E+01	1.04E+02		1.08E+06					
8	Container plastic	162	1.3E+01	2.24E+01		2.32E+05					
9	Total Cellulosics			237.61591	1.8E+04	3.3E+06	4.19E+06	1.6E+08	1.55E+08		
10											
11											
12	Wang and Brush (1996)										
13											
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
15											
16	162 g/mol was used for all cellulose										
17											
18	PA parameter data base										
19	Total volume of CH waste			1.69E+05							
20	Ratio factor for one panel			0.1044							
21	Total volume of CH waste for ONE panel			1.76E+04							

RH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Letter 2003, Waste Material Parameter Disposal Inventory					Average drum of RH waste for one panel					
2											
3		Formula	Avg Density	Cellulosic	volume	weight	weight for	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	one panel	of C	of CO2		
5	Cellulosics	162	6.1	6.1							
6	Rubber	162	3.6	3.6							
7	Plastics	162	7	11.9							
8	Total Cellulosics			2.25504	7.4E+02	1.7E+03	174.01573	6.4E+03	6.4E+03		
9											
10											
11	Wang and Brush (1996)										
12											
13	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence:										Q=1.7P+R
14											
15	162 g/mol was used for all cellulosics										
16											
17	PA parameter data base										
18	Total volume of RH waste		7.08E+03								

Safety Factor

	A	B	C	D	E	F	G	H	I	J	K
1											
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.										
3											
4			Volume								
5		Moles	m3								
6	Mg dissolved	1.06E+06									
7	Max CO2 generated	1.55E+08									
8	Max CO2 (RH)	6.45E+03									
9	Total MgO required	1.56E+08	3.93E+03								
10											
11								Ratio factor from sheet "PA supersack ratio" row 16:		1.095	
12	Total MgO currently being emplaced in WIPP										
13								Total Metric Tons of MgO is from Marcinowski, 2001			
14	Tons	Kg	g	moles	85% react			7.40E+04	short tons		
15	7.67E+03	7674487.43	7.67E+09	1.90E+08	1.61E+08			9.07E-01	conversion factor		
16								6.71E+04	metric tons		
17											
18											
19	Safety Factor with new inventory data assuming one mole of C produces one mole CO2										
20											
21	Safety Factor		1.03E+00								

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APPENDIX H: SNL54CPRpaneIX.XLS

MgO Dissolved in Brine

	A	B	C	D	E	F	G	H	I
1									
2									
3									
4									
5	GWB	Moles of MgO dissolved in brines							
6									
7		Initial and final concs by		EQ3	done by	Yongliang Xiong			
8	Concentration of Mg in brine								
9									
10		Initial Conc	Final Conc in equil	Final Conc					
11		Mol/L	with MgO, mol/Kg	mol/L		Molality to molarity ratio factor			1.146
12	Mg	1.000	7.8996E-01	0.6893194					
13									
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs							
15									
16									
17	Castile	Calculated by EQ3				Molality to molarity ratio factor			1.137
18									
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO			
20		Mol/L	with MgO, mol/Kg	mol/L	m3 *	dissolved			
21	Mg	0.019	1.0044E-01	8.8338E-02	1.46E+05	1.01E+07			
22									
23									
24									
25									
26									
27									
28									
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000- yrs) in BRAGFLO								

SL

PA Supersack Ratio

	A	B	C	D	E	F	G	H
1								
2		PER PANEL						
3	Case 1	PA						operational
4		12082		seven packs				10908
5		3		seven packs per available space				
6		4027.333		supersacks				3636
7		16914800		Mass of MgO (lb) per panel				
8		7672425		Mass of MgO (kg) per panel				
9								
10	Case 2	operational						
11		67132800		Mass of MgO (kg) currently scheduled to be emplaced				
12		0.1044		Ratio factor for one PA panel				
13		7008664		Mass of MgO (kg) emplaced in one panel				
14		3678.919		supersacks of MgO in one PA panel				
15								
16	Ratio	1.094706						
17	# supersacks							
18								
19		supersack		4200	lb			
20		number in one panel		1905	kg			
21								
22								
23								
24								
25		Safety Factor corresponds to one supersack per stack.						

ST

CH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Average drum of CH waste for panel X assuming 54% of the containers originated from INEEL										
2	Cellulosic numbers given by C. Leigh										
3		Formula	Avg Density	Cellulosic	volume	weight	weight (kg)	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	cell equivalent	of C	of CO2		
5	Cellulosics	162	8.8E+01	8.84E+01		1.56E+06					
6	Rubber	162	2.3E+01	2.28E+01		4.02E+05					
7	Plastics	162	6.1E+01	1.04E+02		1.08E+06					
8	Container plastic	162	1.3E+01	2.24E+01		2.32E+05					
9	Total Cellulosics			237.61591	1.8E+04	3.3E+06	4.19E+06	1.6E+08	1.6E+08		
10											
11											
12	Wang and Brush (1996)										
13											
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
15											
16	162 g/mol was used for all cellulose										
17											
18	PA parameter data base										
19	Total volume of CH waste			1.69E+05							
20	Ratio factor for one panel			0.1044							
21	Total volume of CH waste for ONE panel			1.76E+04							
22											
23	Moles of Nitrate and Sulfate Initially Present in the Waste					*from "Estimate of Oxyanion in a Single Panel in the WIPP Repository in Support of AP-107 Supercedes ERMS#530988 Rev. 1"					
24											
25		kg*	g	fw	moles						
26	Nitrate (NO3)	2.31E+05	2.31E+08	62.01	3.73E+06						
27	Sulfate (SO4)	1.20E+04	1.20E+07	96.06	1.25E+05						
28											
29											
30	Molar fraction of cellulose biodegraded via denitrification						3.00				
31											
32	Molar fraction of cellulose biodegraded via sulfate reduction						0.16				
33											
34	Molar fraction of cellulose from methanogenesis						96.84				
35											
36					moles						
37	Total CO2 production for the repository					8.01E+07					

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RH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	<u>Letter 2003, Waste Material Parameter Disposal Inventory</u>					Average drum of RH waste for one panel					
2											
3		Formula	Avg Density	Cellulosic	volume	weight	weight for	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	one panel	of C	of CO2		
5	Cellulosics	162	6.1	6.1							
6	Rubber	162	3.6	3.6							
7	Plastics	162	7	11.9							
8	Total Cellulosics			2.25504	7.4E+02	1.7E+03	174.01573	6.4E+03	3.2E+03		
9											
10											
11	<u>Wang and Brush (1996)</u>										
12											
13	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulotics, based on carbon equivalence:										Q=1.7P+R
14											
15	162 g/mol was used for all cellulotics										
16											
17	<u>PA parameter data base</u>										
18	Total volume of RH waste		7.08E+03								

Safety Factor

	A	B	C	D	E	F	G	H	I	J	K
1											
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.										
3											
4			Volume								
5		Moles	m3								
6	Mg dissolved	1.06E+06									
7	Max CO2 generated	8.01E+07									
8	Max CO2 (RH)	3.22E+03									
9	Total MgO required	8.11E+07	2.04E+03								
10											
11											
12	Total MgO currently being emplaced in WIPP						Ratio factor from sheet "PA supersack ratio" row 16:				1.095
13											
14	Tons	Kg	g	moles	85% react		Total Metric Tons of MgO is from Marcinowski, 2001				
15	7.78E+03	7776113.06	7.78E+09	1.93E+08	1.63E+08		7.40E+04	short tons			
16							9.07E-01	conversion factor			
17							6.71E+04	metric tons			
18											
19	Safety Factor with new inventory data assuming one mole of C produces one mole CO2										
20											
21	Safety Factor		2.01E+00								

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APPENDIX I: MgOsafetyfactorSNLPAcalcs.XLS

MgO Dissolved in Brine

	A	B	C	D	E	F	G	H	I
1									
2									
3									
4									
5	GWB	Moles of MgO dissolved in brines							
6		Initial and final concs by			EQ3	done by	Yongliang Xiong		
7									
8	Concentration of Mg in brine								
9									
10		Initial Conc	Final Conc in equil	Final Conc					
11		Mol/L	with MgO, mol/Kg	mol/L			Molality to molarity ratio factor		1.146
12	Mg	1.000	7.8996E-01	0.6893194					
13									
14		GWB ends up with less Mg++ in solution and will be neglected for further calcs							
15									
16									
17	Castile	Calculated by EQ3					Molality to molarity ratio factor		1.137
18									
19		Initial Conc	Final Conc in equil	Final Conc	Volume	Moles of MgO			
20		Mol/L	with MgO, mol/Kg	mol/L	m3 *	dissolved			
21	Mg	0.019	1.0044E-01	8.8338E-02	1.46E+05	1.01E+07			
22									
23									
24									
25									
26									
27									
28									
29	* Max brine flow up the bore hole at the upper DRZ S3 scenario (E1 @ 1000+ yrs) in BRAGFLO								

Conservative Case

	A	B	C	D	E	F	G	H	I	J	K	L	M	
1														
2														
3														
4	Conservative Case													
5			Kilograms						number	m3	m3	%	%	
6	Total		Cellulosics	Plastics	Rubber	Plastic Liners		containers waste	container	waste	of total	of total		
7	Panel X		1.56E+06	1.08E+06	4.02E+05	2.32E+05		for panel X	volume	volume	containers	volume		
8														
9	Per container													
10	SC		114.71	77.52	30.29	0			0.379					
11	TDOP		12.86	16.99	0.04	91.55			4.79					
12	SWB		5.17	6.72	0.02	30.24			1.89					
13	55 gal		7	5.51	1.48	3.73			0.208					
14														
15	Total													
16	SC	INEEL	1.45E+06	9.77E+05	3.82E+05	0.00E+00		12603		4776.537	44.3	27.5	84.2	
17	TDOP	INEEL	2.17E+04	2.87E+04	6.76E+01	1.55E+05		1691		8099.89	5.95	46.6		
18	SWB	INEEL	4.77E+03	6.20E+03	1.84E+01	2.79E+04		922		1742.58	3.24	10.0		
19	55 gal		9.25E+04	7.28E+04	1.95E+04	4.93E+04		13208		2747.264	46.5	15.8	15.8	
20														
21	Check	Total	1.56E+06	1.08E+06	4.01E+05	2.32E+05		2.84E+04		17366.27				
22														
23	Total	INEEL	1.47E+06	1.01E+06	3.82E+05	1.83E+05								
24														
25														
26														
27			Kilograms						number					
28	Total		Nitrates	Sulfates				containers waste						
29	Panel X		2.31E+05	1.20E+04				for panel X						
30														
31	Per container													
32	SC		0	0										
33	TDOP		91.16	1.22										
34	SWB		36.08	0.6										
35	55 gal		3.31	0.71										
36														
37	Total													
38	SC	INEEL	0.00E+00	0.00E+00				12603						
39	TDOP	INEEL	1.54E+05	2.06E+03				1691						
40	SWB	INEEL	3.33E+04	5.53E+02				922						
41	55 gal		4.37E+04	9.38E+03				13208						
42														
43	Check	Total	2.31E+05	1.20E+04				2.84E+04						
44														
45	Total	INEEL	1.87E+05	2.62E+03										

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CH CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Average drum of CH waste (no INEEL) for 46% of panel X										
2											
3		Formula	Avg Density	Cellulosic	volume	weight	equivalent cell wt	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	Kg	of C	of CO2		
5	Cellulosics	162	5.24E+00	5.24E+00		9.25E+04					
6	Rubber	162	1.11E+00	1.11E+00		1.95E+04					
7	Plastics	162	4.13E+00	7.01E+00		7.28E+04					
8	Container plastic	162	2.79E+00	4.75E+00		4.93E+04					
9	Total Cellulosics			18.112517	1.8E+04	3.2E+05	3.20E+05	1.2E+07	2E+07		
10											
11											
12	<u>Wang and Brush (1996)</u>										
13											
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulosics, based on carbon equivalence:										Q=1.7P+R
15											
16	162 g/mol was used for all cellulosics										
17											
18	<u>PA parameter data base</u>										
19	Total volume of CH waste			1.69E+05							
20											
21											
22											
23	Moles of Nitrate and Sulfate Initially Present in the Waste										
24											
25		kg*	g	fw	moles						
26	Nitrate (NO3)	4.37E+04	4.37E+07	62.01	7.05E+05						
27	Sulfate (SO4)	9.38E+03	9.38E+06	96.06	9.76E+04						
28											
29											
30	<u>Molar fraction of cellulosics biodegraded via denitrification</u>							7.44			
31											
32	<u>Molar fraction of cellulosics biodegraded via sulfate reduction</u>							1.65			
33											
34	<u>Molar fraction of cellulosics from methanogenesis</u>							90.91			
35											
36					moles						
37	Total CO2 production for the repository						6.5E+06				

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INEEL CPR

	A	B	C	D	E	F	G	H	I	J	K
1	Average drum of INEEL CH waste for 54% of panel X										
2											
3		Formula	Avg Density	Cellulosic	volume	weight	equil cell wt	Total moles	Total moles		
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	Kg	of C	of CO2		
5	Cellulosics	162	8.33E+01	8.33E+01		1.47E+06					
6	Rubber	162	2.17E+01	2.17E+01		3.82E+05					
7	Plastics	162	5.72E+01	9.73E+01		1.01E+06					
8	Container plastic	162	1.04E+01	1.76E+01		1.83E+05					
9	Total Cellulosics			2.20E+02	1.8E+04	3.9E+06	3.88E+06	1.4E+08	1.4E+08		
10											
11											
12	Wang and Brush (1996)										
13											
14	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
15											
16	162 g/mol was used for all cellulose										
17											
18	PA parameter data base										
19	Total volume of CH waste			1.69E+05							
20											
21											
22	one mole of C = one half mole of CO2										
23											
24											
25											
26	Moles of Nitrate and Sulfate Initially Present in the Waste										
27											
28		kg*	g	fw	moles						
29	Nitrate (NO3)	1.87E+05	1.87E+08	62.01	3.02E+06						
30	Sulfate (SO4)	2.62E+03	2.62E+06	96.06	2.73E+04						
31											
32							fraction %				
33	Molar fraction of cellulose biodegraded via denitrification						2.62				
34											
35	Molar fraction of cellulose biodegraded via sulfate reduction						0.04				
36											
37	Molar fraction of cellulose from methanogenesis						97.34				
38											
39					moles						
40	Total CO2 production for the repository					7.4E+07					

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RH CPTC

	A	B	C	D	E	F	G	H	I	J	K
1	Letter 2003, Waste Material Parameter Disposal Inventory					Average drum of RH waste					
2											
3		Formula	Avg Density	Cellulosic	volume	weight	Total moles	Total moles			
4		Wt (g/mol)	(Kg/m3)	equivalent	m3	kg	of C	of CO2			
5	Cellulosics	162	4.5	4.5							
6	Rubber	162	3.1	3.1							
7	Plastics	162	6.3	10.71							
8	Total Cellulosics			18.31	7.4E+02	1.4E+04	5.0E+05	2.5E+05			
9											
10											
11	Wang and Brush (1996)										
12											
13	P kg of plastics and R kilograms of rubbers are equivalent to the Q kilograms of cellulose, based on carbon equivalence:										Q=1.7P+R
14											
15	162 g/mol was used for all cellulose										
16											
17	PA parameter data base										
18	Total volume of RH waste		7.08E+03								

Information Only

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Safety Factor

	A	B	C	D	E	F	G	H	I
1									
2	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.								
3									
4			Volume						
5		Moles	m3						
6	Mg dissolved	1.06E+06							
7	Max CO2 without INEEL (46%)	6.46E+06							
8	Max CO2 INEEL (54%)	7.38E+07			Total Metric Tons of MgO is from Marcinowski, 2001				
9	Mas CO2 (RH)	2.51E+05			7.40E+04	short tons			
10	Total MgO required	8.15E+07	2.05E+08		9.07E-01	conversion factor			
11					6.71E+04	metric tons			
12									
13	Total MgO currently being emplaced in WIPP								
14									
15		Tons	Kg	g	moles	85% react			
16	Total repository	6.71E+04	67132800	6.71E+10	1.67E+09	1.41E+09			
17	Panel X	7008.66432	7008664	7.01E+09	1.74E+08	1.47E+08			
18									
19									
20	Safety Factor with new inventory data assuming one mole of C produces one/half mole CO2								
21									
22	Safety Factor		1.80E+00						

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PA Request (EPA)

	A	B	C	D	E	F	G	H	I
1									
2	PER ONE PA PANEL								
3									
4									
5	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity.								
6	Assumes one mole of C = 1/2 mole of CO2								
7									
8			Volume						
9		Moles	m3						
10	Mg dissolved	1.06E+06							
11	Max CO2 without INEEL (46%)	1.18E+07							
12	Max CO2 INEEL (54%)	1.44E+08							
13	Max CO2 RH	2.51E+05							
14	Total MgO required	1.57E+08							
15				Tons	kg	g	moles	moles *85%	
16	Total MgO currently being emplaced in WIPP			6.71E+04	67132800	6.71E+10	1.67E+09	1.41E+09	
17									
18	Total MgO for one PA panel			7008.66432	7008664.32	7.01E+09	1.74E+08	1.47E+08	
19									
20		Safety Factor		9.38E-01					
21									
22									
23	Data for following table calculations								
24									
25	Given								
26	cellulosic density			36.42	kg/m3				
27	Super sack volume			47.60	ft3	1.35E+00	m3		
28	MgO mass per sack			4200.00	lb	1.91E+06	g		
29	Super sack density			1413395.25	g/m3				
30	panel CH volume			17643.60	m3				
31									
32									
33									
34									
35									
36									
37									
38									
39									
40									
41									
42									
43									
44							Currently	Total	
45	Waste without INEEL	Scaled %	INEEL	Scaled %	Waste without INEEL	INEEL	emplaced	MgO	
46	m3		m3		moles	moles	MgO mol	moles	
47	1	6.33	0	0	7.49E+07	0.00E+00	1.47E+08	7.62E+07	1.93E+00
48	0.99	6.27	0.01	0.01	7.42E+07	1.71E+06	1.47E+08	7.72E+07	1.91E+00
49	0.98	6.20	0.02	0.02	7.34E+07	3.41E+06	1.47E+08	7.81E+07	1.88E+00
50	0.97	6.14	0.03	0.04	7.27E+07	5.12E+06	1.47E+08	7.91E+07	1.86E+00
51	0.96	6.08	0.04	0.05	7.19E+07	6.83E+06	1.47E+08	8.00E+07	1.84E+00
52	0.95	6.01	0.05	0.06	7.12E+07	8.53E+06	1.47E+08	8.10E+07	1.82E+00

Information Only

PA Request (EPA) continued

	A	B	C	D	E	F	G	H	I
45	Waste without INEEL	Scaled %	INEEL	Scaled %	Waste without INEEL	INEEL	emplaced	MgO	Safety
46	m3		m3		moles	moles	MgO mol	moles	Factor
53	0.94	5.95	0.06	0.07	7.04E+07	1.02E+07	1.47E+08	8.20E+07	1.80E+00
54	0.93	5.89	0.07	0.08	6.97E+07	1.19E+07	1.47E+08	8.29E+07	1.77E+00
55	0.92	5.82	0.08	0.10	6.89E+07	1.37E+07	1.47E+08	8.39E+07	1.75E+00
56	0.91	5.76	0.09	0.11	6.82E+07	1.54E+07	1.47E+08	8.48E+07	1.73E+00
57	0.9	5.70	0.1	0.12	6.74E+07	1.71E+07	1.47E+08	8.58E+07	1.71E+00
58	0.89	5.63	0.11	0.13	6.67E+07	1.88E+07	1.47E+08	8.68E+07	1.70E+00
59	0.88	5.57	0.12	0.14	6.59E+07	2.05E+07	1.47E+08	8.77E+07	1.68E+00
60	0.87	5.51	0.13	0.15	6.52E+07	2.22E+07	1.47E+08	8.87E+07	1.66E+00
61	0.86	5.44	0.14	0.17	6.44E+07	2.39E+07	1.47E+08	8.96E+07	1.64E+00
62	0.85	5.38	0.15	0.18	6.37E+07	2.56E+07	1.47E+08	9.06E+07	1.62E+00
63	0.84	5.32	0.16	0.19	6.29E+07	2.73E+07	1.47E+08	9.15E+07	1.61E+00
64	0.83	5.25	0.17	0.20	6.22E+07	2.90E+07	1.47E+08	9.25E+07	1.59E+00
65	0.82	5.19	0.18	0.21	6.14E+07	3.07E+07	1.47E+08	9.35E+07	1.57E+00
66	0.81	5.13	0.19	0.23	6.07E+07	3.24E+07	1.47E+08	9.44E+07	1.56E+00
67	0.8	5.06	0.2	0.24	5.99E+07	3.41E+07	1.47E+08	9.54E+07	1.54E+00
68	0.79	5.00	0.21	0.25	5.92E+07	3.58E+07	1.47E+08	9.63E+07	1.53E+00
69	0.78	4.94	0.22	0.26	5.84E+07	3.75E+07	1.47E+08	9.73E+07	1.51E+00
70	0.77	4.87	0.23	0.27	5.77E+07	3.93E+07	1.47E+08	9.82E+07	1.50E+00
71	0.76	4.81	0.24	0.29	5.69E+07	4.10E+07	1.47E+08	9.92E+07	1.48E+00
72	0.75	4.75	0.25	0.30	5.62E+07	4.27E+07	1.47E+08	1.00E+08	1.47E+00
73	0.74	4.68	0.26	0.31	5.54E+07	4.44E+07	1.47E+08	1.01E+08	1.46E+00
74	0.73	4.62	0.27	0.32	5.47E+07	4.61E+07	1.47E+08	1.02E+08	1.44E+00
75	0.72	4.56	0.28	0.33	5.39E+07	4.78E+07	1.47E+08	1.03E+08	1.43E+00
76	0.71	4.49	0.29	0.34	5.32E+07	4.95E+07	1.47E+08	1.04E+08	1.41E+00
77	0.7	4.43	0.3	0.36	5.24E+07	5.12E+07	1.47E+08	1.05E+08	1.40E+00
78	0.69	4.37	0.31	0.37	5.17E+07	5.29E+07	1.47E+08	1.06E+08	1.39E+00
79	0.68	4.30	0.32	0.38	5.09E+07	5.46E+07	1.47E+08	1.07E+08	1.38E+00
80	0.67	4.24	0.33	0.39	5.02E+07	5.63E+07	1.47E+08	1.08E+08	1.36E+00
81	0.66	4.18	0.34	0.40	4.94E+07	5.80E+07	1.47E+08	1.09E+08	1.35E+00
82	0.65	4.11	0.35	0.42	4.87E+07	5.97E+07	1.47E+08	1.10E+08	1.34E+00
83	0.64	4.05	0.36	0.43	4.79E+07	6.14E+07	1.47E+08	1.11E+08	1.33E+00
84	0.63	3.99	0.37	0.44	4.72E+07	6.31E+07	1.47E+08	1.12E+08	1.32E+00
85	0.62	3.92	0.38	0.45	4.64E+07	6.49E+07	1.47E+08	1.13E+08	1.31E+00
86	0.61	3.86	0.39	0.46	4.57E+07	6.66E+07	1.47E+08	1.14E+08	1.30E+00
87	0.6	3.80	0.4	0.48	4.49E+07	6.83E+07	1.47E+08	1.15E+08	1.28E+00
88	0.59	3.73	0.41	0.49	4.42E+07	7.00E+07	1.47E+08	1.15E+08	1.27E+00
89	0.58	3.67	0.42	0.50	4.34E+07	7.17E+07	1.47E+08	1.16E+08	1.26E+00
90	0.57	3.61	0.43	0.51	4.27E+07	7.34E+07	1.47E+08	1.17E+08	1.25E+00
91	0.56	3.54	0.44	0.52	4.20E+07	7.51E+07	1.47E+08	1.18E+08	1.24E+00
92	0.55	3.48	0.45	0.53	4.12E+07	7.68E+07	1.47E+08	1.19E+08	1.23E+00
93	0.54	3.42	0.46	0.55	4.05E+07	7.85E+07	1.47E+08	1.20E+08	1.22E+00
94	0.53	3.35	0.47	0.56	3.97E+07	8.02E+07	1.47E+08	1.21E+08	1.21E+00
95	0.52	3.29	0.48	0.57	3.90E+07	8.19E+07	1.47E+08	1.22E+08	1.20E+00
96	0.51	3.23	0.49	0.58	3.82E+07	8.36E+07	1.47E+08	1.23E+08	1.19E+00
97	0.5	3.16	0.5	0.59	3.75E+07	8.53E+07	1.47E+08	1.24E+08	1.19E+00
98	0.49	3.10	0.51	0.61	3.67E+07	8.70E+07	1.47E+08	1.25E+08	1.18E+00
99	0.48	3.04	0.52	0.62	3.60E+07	8.88E+07	1.47E+08	1.26E+08	1.17E+00
100	0.47	2.97	0.53	0.63	3.52E+07	9.05E+07	1.47E+08	1.27E+08	1.16E+00
101	0.46	2.91	0.54	0.64	3.45E+07	9.22E+07	1.47E+08	1.28E+08	1.15E+00
102	0.45	2.85	0.55	0.65	3.37E+07	9.39E+07	1.47E+08	1.29E+08	1.14E+00

PA Request (EPA) continued

	A	B	C	D	E	F	G	H	I
45	Waste without INEEL	Scaled %	INEEL	Scaled %	Waste without INEEL	INEEL	emplaced	MgO	
46	mg		mg		moles	moles	MgO mol	moles	
103	0.44	2.78	0.56	0.67	3.30E+07	9.56E+07	1.47E+08	1.30E+08	1.13E+00
104	0.43	2.72	0.57	0.68	3.22E+07	9.73E+07	1.47E+08	1.31E+08	1.12E+00
105	0.42	2.66	0.58	0.69	3.15E+07	9.90E+07	1.47E+08	1.32E+08	1.12E+00
106	0.41	2.59	0.59	0.70	3.07E+07	1.01E+08	1.47E+08	1.33E+08	1.11E+00
107	0.4	2.53	0.6	0.71	3.00E+07	1.02E+08	1.47E+08	1.34E+08	1.10E+00
108	0.39	2.47	0.61	0.72	2.92E+07	1.04E+08	1.47E+08	1.35E+08	1.09E+00
109	0.38	2.41	0.62	0.74	2.85E+07	1.06E+08	1.47E+08	1.36E+08	1.09E+00
110	0.37	2.34	0.63	0.75	2.77E+07	1.08E+08	1.47E+08	1.37E+08	1.08E+00
111	0.36	2.28	0.64	0.76	2.70E+07	1.09E+08	1.47E+08	1.38E+08	1.07E+00
112	0.35	2.22	0.65	0.77	2.62E+07	1.11E+08	1.47E+08	1.38E+08	1.06E+00
113	0.34	2.15	0.66	0.78	2.55E+07	1.13E+08	1.47E+08	1.39E+08	1.06E+00
114	0.33	2.09	0.67	0.80	2.47E+07	1.14E+08	1.47E+08	1.40E+08	1.05E+00
115	0.32	2.03	0.68	0.81	2.40E+07	1.16E+08	1.47E+08	1.41E+08	1.04E+00
116	0.31	1.96	0.69	0.82	2.32E+07	1.18E+08	1.47E+08	1.42E+08	1.03E+00
117	0.3	1.90	0.7	0.83	2.25E+07	1.19E+08	1.47E+08	1.43E+08	1.03E+00
118	0.29	1.84	0.71	0.84	2.17E+07	1.21E+08	1.47E+08	1.44E+08	1.02E+00
119	0.28	1.77	0.72	0.86	2.10E+07	1.23E+08	1.47E+08	1.45E+08	1.01E+00
120	0.27	1.71	0.73	0.87	2.02E+07	1.25E+08	1.47E+08	1.46E+08	1.01E+00
121	0.26	1.65	0.74	0.88	1.95E+07	1.26E+08	1.47E+08	1.47E+08	1.00E+00
122	0.25	1.58	0.75	0.89	1.87E+07	1.28E+08	1.47E+08	1.48E+08	9.94E-01
123	0.24	1.52	0.76	0.90	1.80E+07	1.30E+08	1.47E+08	1.49E+08	9.87E-01
124	0.23	1.46	0.77	0.91	1.72E+07	1.31E+08	1.47E+08	1.50E+08	9.81E-01
125	0.22	1.39	0.78	0.93	1.65E+07	1.33E+08	1.47E+08	1.51E+08	9.75E-01
126	0.21	1.33	0.79	0.94	1.57E+07	1.35E+08	1.47E+08	1.52E+08	9.69E-01
127	0.2	1.27	0.8	0.95	1.50E+07	1.37E+08	1.47E+08	1.53E+08	9.63E-01
128	0.19	1.20	0.81	0.96	1.42E+07	1.38E+08	1.47E+08	1.54E+08	9.57E-01
129	0.18	1.14	0.82	0.97	1.35E+07	1.40E+08	1.47E+08	1.55E+08	9.51E-01
130	0.17	1.08	0.83	0.99	1.27E+07	1.42E+08	1.47E+08	1.56E+08	9.45E-01
131	0.158	1	0.842	1	1.18E+07	1.44E+08	1.47E+08	1.57E+08	9.38E-01
132	0.15	0.95	0.85	1.01	1.12E+07	1.45E+08	1.47E+08	1.58E+08	9.33E-01
133	0.14	0.89	0.86	1.02	1.05E+07	1.47E+08	1.47E+08	1.59E+08	9.28E-01
134	0.13	0.82	0.87	1.03	9.74E+06	1.48E+08	1.47E+08	1.60E+08	9.22E-01
135	0.12	0.76	0.88	1.05	8.99E+06	1.50E+08	1.47E+08	1.60E+08	9.17E-01
136	0.11	0.70	0.89	1.06	8.24E+06	1.52E+08	1.47E+08	1.61E+08	9.11E-01
137	0.1	0.63	0.9	1.07	7.49E+06	1.54E+08	1.47E+08	1.62E+08	9.06E-01
138	0.09	0.57	0.91	1.08	6.74E+06	1.55E+08	1.47E+08	1.63E+08	9.01E-01
139	0.08	0.51	0.92	1.09	5.99E+06	1.57E+08	1.47E+08	1.64E+08	8.95E-01
140	0.07	0.44	0.93	1.10	5.24E+06	1.59E+08	1.47E+08	1.65E+08	8.90E-01
141	0.06	0.38	0.94	1.12	4.49E+06	1.60E+08	1.47E+08	1.66E+08	8.85E-01
142	0.05	0.32	0.95	1.13	3.75E+06	1.62E+08	1.47E+08	1.67E+08	8.80E-01
143	0.04	0.25	0.96	1.14	3.00E+06	1.64E+08	1.47E+08	1.68E+08	8.75E-01
144	0.03	0.19	0.97	1.15	2.25E+06	1.66E+08	1.47E+08	1.69E+08	8.70E-01
145	0.02	0.13	0.98	1.16	1.50E+06	1.67E+08	1.47E+08	1.70E+08	8.65E-01
146	0.01	0.06	0.99	1.18	7.49E+05	1.69E+08	1.47E+08	1.71E+08	8.60E-01
147	0	0	1	1.19	0.00E+00	1.71E+08	1.47E+08	1.72E+08	8.56E-01

PA Request (DOE)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	PER ONE PA PANEL																		
2																			
3																			
4																			
5	Total MgO required for dissolving in brine and reacting with CO2 generated by microbial activity																		
6	Assume one mole of C = 1/2 mole of CO2																		
7																			
8																			
9																			
10	Mg dissolved	1.06E+06																	
11	Max CO2 without INEEL (46%)	6.48E+06																	
12	Max CO2 INEEL (84%)	7.39E+07																	
13	Max CO2 RH	2.51E+05																	
14	Total MgO required	8.19E+07																	
15																			
16	Total MgO currently being employed in WIPP	6.71E+04			6.71E+04		6.71E+10		1.67E+09		1.41E+09								
17																			
18	Total MgO for one PA panel	7008.65432			7008664.32		7.01E+09		1.74E+08		1.47E+08								
19																			
20	Safety Factor	1.90E+00																	
21																			
22																			
23	Data for following table calculations																		
24																			
25	QWIP																		
26	solubility density	36.42			kg/m3		1.35E+00												
27	Super sack volume	47.60			ft3														
28	MgO mass per sack	4200.00			lb		1.91E+06												
29	Super sack density	1413396.25			g/m3														
30	panel CH volume	17643.60			m3														
31																			
32	Moles of Nitrate and Sulfate Initially Present in the Waste																		
33																			
34	CH without INEEL	kg			moles		INEEL		kg		g		hr		moles				
35	Nitrate (NO3)	4.37E+04		4.37E+07	52.01		7.05E+05		Nitrate (NO3)	1.87E+05		1.87E+08		62.01		3.02E+08			
36	Sulfate (SO4)	2.38E+03		9.38E+06	96.08		8.78E+04		Sulfate (SO4)	2.62E+03		2.62E+06		96.08		2.79E+04			
37																			
38																			
39																			
40	Table																		
41																			
42																			
43																			
44																			
45	Waste without INEEL	Scaled %	INEEL	Scaled %	Waste without INEEL	INEEL	original moles of CO2 produced before Nitrate, Sulfate, and methanogenesis	Fraction % denitrification	Fraction % sulfate reduction	Fraction % methanogenesis	Nitrate & Sulfate effect on INEEL	original moles of CO2 produced before Nitrate, Sulfate, and methanogenesis	Fraction % denitrification	Fraction % sulfate reduction	Fraction % methanogenesis	Nitrate & Sulfate effect on INEEL	Currently employed MgO mol	Total MgO moles	
46	mg		mg		moles	moles													
47	0.98	4.98	0.02	0.02	3.99E+07	2.63E+06	7.27E+07	1.21	0.27	96.52	3.7E+07	3.12E+06	73.62	1.07	25.31	4.5E+06	1.47E+08	4.28E+07	3.45E+08
48	0.99	5.27	0.01	0.01	3.92E+07	2.50E+06	7.19E+07	1.22	0.27	96.50	3.6E+07	6.89E+06	55.22	0.80	43.99	5.3E+06	1.47E+08	4.31E+07	3.41E+08
49	0.98	5.20	0.02	0.02	3.88E+07	2.58E+06	7.12E+07	1.24	0.27	96.49	3.6E+07	5.93E+06	44.17	0.64	35.19	6.2E+06	1.47E+08	4.36E+07	3.37E+08
50	0.97	6.04	0.03	0.04	3.99E+07	2.63E+06	7.27E+07	1.21	0.27	96.52	3.7E+07	3.12E+06	73.62	1.07	25.31	4.5E+06	1.47E+08	4.28E+07	3.45E+08
51	0.96	6.18	0.04	0.05	3.92E+07	2.50E+06	7.19E+07	1.22	0.27	96.50	3.6E+07	6.89E+06	55.22	0.80	43.99	5.3E+06	1.47E+08	4.31E+07	3.41E+08
52	0.95	6.01	0.05	0.06	3.88E+07	2.58E+06	7.12E+07	1.24	0.27	96.49	3.6E+07	5.93E+06	44.17	0.64	35.19	6.2E+06	1.47E+08	4.36E+07	3.37E+08
53	0.94	5.95	0.06	0.07	3.84E+07	2.52E+06	7.04E+07	1.25	0.28	96.47	3.6E+07	1.02E+07	36.81	0.53	62.66	7.0E+06	1.47E+08	4.41E+07	3.34E+08
54	0.93	5.89	0.07	0.08	3.80E+07	2.46E+06	6.97E+07	1.26	0.28	96.46	3.6E+07	1.19E+07	31.55	0.48	67.99	7.9E+06	1.47E+08	4.46E+07	3.30E+08
55	0.92	5.82	0.08	0.10	3.76E+07	2.40E+06	6.89E+07	1.28	0.28	96.44	3.5E+07	1.37E+07	27.51	0.40	71.99	8.7E+06	1.47E+08	4.50E+07	3.27E+08
56	0.91	5.76	0.09	0.11	3.72E+07	2.34E+06	6.82E+07	1.29	0.29	96.42	3.5E+07	1.54E+07	24.54	0.36	75.10	9.6E+06	1.47E+08	4.55E+07	3.23E+08
57	0.9	5.70	0.1	0.12	3.68E+07	2.28E+06	6.74E+07	1.31	0.29	96.40	3.4E+07	1.71E+07	22.09	0.32	77.53	1.0E+07	1.47E+08	4.60E+07	3.20E+08
58	0.89	5.63	0.11	0.13	3.64E+07	2.22E+06	6.67E+07	1.32	0.29	96.38	3.4E+07	1.88E+07	20.08	0.29	79.53	1.1E+07	1.47E+08	4.65E+07	3.17E+08
59	0.88	5.57	0.12	0.14	3.60E+07	2.16E+06	6.60E+07	1.34	0.30	96.37	3.3E+07	2.05E+07	18.41	0.27	81.33	1.2E+07	1.47E+08	4.70E+07	3.13E+08
60	0.87	5.51	0.13	0.16	3.55E+07	2.10E+06	6.52E+07	1.35	0.30	96.35	3.3E+07	2.22E+07	16.29	0.25	82.76	1.3E+07	1.47E+08	4.74E+07	3.10E+08
61	0.86	5.44	0.14	0.17	3.51E+07	2.04E+06	6.44E+07	1.37	0.30	96.33	3.3E+07	2.39E+07	15.78	0.23	84.00	1.4E+07	1.47E+08	4.79E+07	3.07E+08
62	0.85	5.38	0.15	0.18	3.47E+07	1.98E+06	6.37E+07	1.38	0.31	96.31	3.2E+07	2.56E+07	14.72	0.21	85.06	1.5E+07	1.47E+08	4.84E+07	3.04E+08
63	0.84	5.32	0.16	0.19	3.43E+07	1.92E+06	6.29E+07	1.40	0.31	96.29	3.2E+07	2.73E+07	13.80	0.20	86.00	1.6E+07	1.47E+08	4.89E+07	3.01E+08
64	0.83	5.26	0.17	0.20	3.39E+07	1.86E+06	6.22E+07	1.42	0.31	96.27	3.2E+07	2.90E+07	12.99	0.19	86.82	1.6E+07	1.47E+08	4.94E+07	2.98E+08
65	0.82	5.19	0.18	0.21	3.35E+07	1.80E+06	6.14E+07	1.43	0.32	96.25	3.1E+07	3.07E+07	12.27	0.18	87.55	1.7E+07	1.47E+08	4.99E+07	2.95E+08
66	0.81	5.13	0.19	0.23	3.31E+07	1.74E+06	6.07E+07	1.45	0.32	96.23	3.1E+07	3.24E+07	11.62	0.17	88.11	1.8E+07	1.47E+08	5.03E+07	2.92E+08
67	0.8	5.06	0.2	0.24	3.27E+07	1.68E+06	5.99E+07	1.47	0.33	96.20	3.1E+07	3.41E+07	11.04	0.16	88.82	1.9E+07	1.47E+08	5.08E+07	2.89E+08
68	0.79	5.00	0.21	0.25	3.23E+07	1.62E+06	5.92E+07	1.49	0.33	96.18	3.0E+07	3.58E+07	10.52	0.16	89.33	2.0E+07	1.47E+08	5.13E+07	2.87E+08
69	0.78	4.94	0.22	0.26	3.19E+07	1.56E+06	5.84E+07	1.51	0.33	96.16	3.0E+07	3.75E+07	10.04	0.16	89.82	2.1E+07	1.47E+08	5.17E+07	2.84E+08
70	0.77	4.87	0.23	0.27	3.15E+07	2.01E+07	5.77E+07	1.53	0.34	96.13	2.9E+07	3.92E+07	9.60	0.14	90.26	2.2E+07	1.47E+08	5.22E+07	2.82E+08
71	0.76	4.81	0.24	0.29	3.11E+07	2.10E+07	5.69E+07	1.55	0.34	96.11	2.9E+07	4.10E+07	9.20	0.13	90.66	2.2E+07	1.47E+08	5.27E+07	2.79E+08
72	0.75	4.75	0.25	0.30	3.07E+07	2.19E+07	5.62E+07	1.57	0.35	96.08	2.8E+07	4.27E+07	8.83	0.13	91.04	2.3E+07	1.47E+08	5.32E+07	2.77E+08
73	0.74	4.68	0.26	0.31	3.02E+07	2.28E+07	5.54E+07	1.59	0.35	96.06	2.8E+07	4.44E+07	8.43	0.12	91.36	2.4E+07	1.47E+08	5.37E+07	2.74E+08
74	0.73	4.62	0.27	0.32	2.98E+07	2.37E+07	5.47E+07	1.61	0.36	96.03	2.8E+07	4.61E+07	8.18	0.12	91.70	2.5E+07	1.47E+08	5.41E+07	2.72E+08
75	0.72	4.56	0.28	0.33	2.94E+07	2.45E+07	5.39E+07	1.63	0.36	96.00	2.8E+07	4.78E+07	7.89	0.11	92.00	2.6E+07	1.47E+08	5.46E+07	2.69E+08
76	0.71	4.49	0.29	0.34	2.90E+07	2.54E+07	5.32E+07	1.65	0.37	95.97	2.7E+07	4.95E+07	7.62	0.11	92.27	2.7E+07	1.47E+08	5.51E+07	2.67E+08
77	0.7	4.43	0.3	0.35	2.86E+07	2.63E+07	5.24E+07	1.68	0.37	95.95									

PA REQUEST (DOE) continued

42	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
43							original moles of CO2 produced before Nitrate, Sulfate, and methanogenesis	Fraction % denitrifier	Fraction % sulfur-oxidizer	Fraction % methanotroph	Nitrate & Sulfate used on mass without INEEL	original moles of CO2 produced before Nitrate, Sulfate, and methanogenesis	Fraction % denitrifier	Fraction % sulfate-reducer	Fraction % methanotroph	Nitrate & Sulfate afford on total	Currently employed MFC (mM)	Total MFC (mM)	
44	Waste without INEEL	Scaled %	INEEL	Scaled %	Waste without INEEL	INEEL					Waste without INEEL								
45																			
46	0.55	3.48	0.46	0.63	2.25E+07	3.94E+07	4.12E+07	2.14	0.47	97.29	2.1E+07	7.65E+07	4.31	0.07	95.02	4.0E+07	1.47E+08	8.28E+07	2.24E+08
47	0.54	3.42	0.46	0.56	2.21E+07	4.05E+07	4.05E+07	2.19	0.48	97.24	2.1E+07	7.65E+07	4.30	0.07	95.13	4.1E+07	1.47E+08	8.30E+07	2.23E+08
48	0.53	3.35	0.47	0.56	2.17E+07	4.12E+07	3.87E+07	2.22	0.49	97.29	2.0E+07	8.02E+07	4.70	0.07	96.29	4.2E+07	1.47E+08	8.37E+07	2.21E+08
49	0.52	3.29	0.48	0.57	2.12E+07	4.21E+07	3.80E+07	2.26	0.50	97.24	2.0E+07	8.19E+07	4.60	0.07	96.39	4.3E+07	1.47E+08	8.42E+07	2.22E+08
50	0.51	3.23	0.49	0.58	2.08E+07	4.29E+07	3.82E+07	2.31	0.51	97.18	2.0E+07	8.38E+07	4.51	0.07	95.49	4.4E+07	1.47E+08	8.47E+07	2.27E+08
51	0.5	3.16	0.5	0.59	2.04E+07	4.36E+07	3.75E+07	2.35	0.52	97.13	1.9E+07	8.55E+07	4.42	0.06	95.52	4.5E+07	1.47E+08	8.52E+07	2.28E+08
52	0.49	3.10	0.51	0.61	2.00E+07	4.47E+07	3.67E+07	2.40	0.53	97.07	1.9E+07	8.70E+07	4.33	0.06	95.61	4.5E+07	1.47E+08	8.56E+07	2.29E+08
53	0.48	3.04	0.52	0.62	1.96E+07	4.59E+07	3.60E+07	2.45	0.54	97.01	1.9E+07	8.89E+07	4.25	0.05	95.69	4.6E+07	1.47E+08	8.61E+07	2.29E+08
54	0.47	2.97	0.53	0.63	1.92E+07	4.64E+07	3.52E+07	2.50	0.55	96.94	1.8E+07	9.06E+07	4.17	0.05	95.77	4.7E+07	1.47E+08	8.65E+07	2.21E+08
55	0.46	2.91	0.54	0.64	1.89E+07	4.73E+07	3.45E+07	2.56	0.57	96.88	1.8E+07	9.22E+07	4.08	0.06	95.85	4.6E+07	1.47E+08	8.71E+07	2.19E+08
56	0.45	2.85	0.55	0.65	1.84E+07	4.82E+07	3.37E+07	2.61	0.58	96.81	1.7E+07	9.39E+07	4.02	0.08	95.93	4.9E+07	1.47E+08	8.75E+07	2.18E+08
57	0.44	2.78	0.56	0.67	1.80E+07	4.91E+07	3.30E+07	2.67	0.59	96.73	1.7E+07	9.56E+07	3.94	0.06	96.00	5.0E+07	1.47E+08	8.80E+07	2.16E+08
58	0.43	2.72	0.57	0.68	1.76E+07	4.99E+07	3.22E+07	2.73	0.61	96.66	1.7E+07	9.73E+07	3.87	0.06	96.07	5.1E+07	1.47E+08	8.85E+07	2.15E+08
59	0.42	2.66	0.58	0.69	1.72E+07	5.17E+07	3.15E+07	2.80	0.62	96.58	1.6E+07	9.90E+07	3.81	0.06	96.14	5.1E+07	1.47E+08	8.90E+07	2.13E+08
60	0.41	2.60	0.59	0.70	1.68E+07	5.17E+07	3.07E+07	2.87	0.64	96.50	1.6E+07	1.01E+08	3.74	0.05	96.20	5.2E+07	1.47E+08	8.95E+07	2.12E+08
61	0.4	2.53	0.6	0.71	1.63E+07	5.26E+07	3.00E+07	2.94	0.65	96.41	1.6E+07	1.02E+08	3.68	0.05	96.27	5.3E+07	1.47E+08	8.99E+07	2.10E+08
62	0.39	2.47	0.61	0.72	1.59E+07	5.34E+07	2.92E+07	3.02	0.67	96.32	1.5E+07	1.04E+08	3.62	0.05	96.39	5.4E+07	1.47E+08	9.04E+07	2.09E+08
63	0.38	2.41	0.62	0.74	1.55E+07	5.43E+07	2.85E+07	3.09	0.69	96.22	1.5E+07	1.06E+08	3.56	0.05	96.39	5.5E+07	1.47E+08	9.09E+07	2.08E+08
64	0.37	2.34	0.63	0.75	1.51E+07	5.52E+07	2.77E+07	3.16	0.70	96.12	1.4E+07	1.08E+08	3.51	0.05	96.44	5.6E+07	1.47E+08	9.14E+07	2.06E+08
65	0.36	2.28	0.64	0.76	1.47E+07	5.61E+07	2.70E+07	3.23	0.72	96.01	1.4E+07	1.09E+08	3.45	0.05	96.50	5.7E+07	1.47E+08	9.19E+07	2.05E+08
66	0.35	2.22	0.65	0.77	1.43E+07	5.69E+07	2.62E+07	3.30	0.74	95.90	1.4E+07	1.11E+08	3.40	0.05	96.55	5.7E+07	1.47E+08	9.23E+07	2.03E+08
67	0.34	2.15	0.66	0.78	1.39E+07	5.78E+07	2.55E+07	3.36	0.77	95.77	1.3E+07	1.13E+08	3.35	0.05	96.61	5.8E+07	1.47E+08	9.28E+07	2.02E+08
68	0.33	2.09	0.67	0.80	1.35E+07	5.87E+07	2.47E+07	3.43	0.79	95.66	1.3E+07	1.14E+08	3.30	0.05	96.66	5.9E+07	1.47E+08	9.33E+07	2.01E+08
69	0.32	2.03	0.68	0.81	1.31E+07	5.96E+07	2.40E+07	3.47	0.81	95.51	1.3E+07	1.16E+08	3.25	0.05	96.71	6.0E+07	1.47E+08	9.38E+07	1.99E+08
70	0.31	1.96	0.69	0.82	1.27E+07	6.04E+07	2.32E+07	3.53	0.84	95.37	1.2E+07	1.18E+08	3.20	0.06	96.75	6.1E+07	1.47E+08	9.43E+07	1.98E+08
71	0.3	1.90	0.7	0.83	1.23E+07	6.13E+07	2.25E+07	3.58	0.87	95.21	1.2E+07	1.19E+08	3.16	0.06	96.80	6.2E+07	1.47E+08	9.47E+07	1.97E+08
72	0.29	1.84	0.71	0.84	1.19E+07	6.22E+07	2.17E+07	3.65	0.90	95.05	1.1E+07	1.21E+08	3.11	0.06	96.84	6.3E+07	1.47E+08	9.52E+07	1.95E+08
73	0.28	1.77	0.72	0.85	1.14E+07	6.31E+07	2.10E+07	3.70	0.93	94.87	1.1E+07	1.23E+08	3.07	0.04	96.89	6.3E+07	1.47E+08	9.57E+07	1.94E+08
74	0.27	1.71	0.73	0.87	1.10E+07	6.40E+07	2.02E+07	3.76	0.97	94.69	1.1E+07	1.25E+08	3.03	0.04	96.93	6.4E+07	1.47E+08	9.62E+07	1.93E+08
75	0.26	1.65	0.74	0.88	1.06E+07	6.48E+07	1.95E+07	3.82	1.00	94.47	1.0E+07	1.26E+08	2.98	0.04	96.97	6.5E+07	1.47E+08	9.67E+07	1.92E+08
76	0.25	1.58	0.75	0.89	1.02E+07	6.57E+07	1.87E+07	3.87	1.04	94.26	9.9E+06	1.28E+08	2.94	0.04	97.01	6.6E+07	1.47E+08	9.71E+07	1.91E+08
77	0.24	1.52	0.76	0.90	9.81E+06	6.66E+07	1.80E+07	3.90	1.09	94.01	9.5E+06	1.30E+08	2.91	0.04	97.05	6.7E+07	1.47E+08	9.76E+07	1.90E+08
78	0.23	1.46	0.77	0.91	9.40E+06	6.75E+07	1.72E+07	3.93	1.13	93.76	9.2E+06	1.31E+08	2.87	0.04	97.09	6.8E+07	1.47E+08	9.81E+07	1.89E+08
79	0.22	1.39	0.78	0.93	8.99E+06	6.83E+07	1.65E+07	3.95	1.19	93.47	8.8E+06	1.33E+08	2.83	0.04	97.13	6.8E+07	1.47E+08	9.85E+07	1.87E+08
80	0.21	1.33	0.79	0.94	8.58E+06	6.92E+07	1.57E+07	3.98	1.24	93.16	8.4E+06	1.35E+08	2.80	0.04	97.16	6.9E+07	1.47E+08	9.90E+07	1.86E+08
81	0.2	1.27	0.8	0.95	8.17E+06	7.01E+07	1.50E+07	3.98	1.30	92.82	8.0E+06	1.37E+08	2.76	0.04	97.20	7.0E+07	1.47E+08	9.95E+07	1.85E+08
82	0.19	1.20	0.81	0.96	7.76E+06	7.10E+07	1.42E+07	3.98	1.37	92.44	7.7E+06	1.39E+08	2.73	0.04	97.23	7.1E+07	1.47E+08	1.00E+08	1.84E+08
83	0.18	1.14	0.82	0.97	7.36E+06	7.18E+07	1.33E+07	3.93	1.45	92.02	7.3E+06	1.40E+08	2.69	0.04	97.27	7.2E+07	1.47E+08	1.00E+08	1.83E+08
84	0.17	1.08	0.83	0.98	6.95E+06	7.27E+07	1.27E+07	3.92	1.53	91.55	6.9E+06	1.42E+08	2.66	0.04	97.30	7.3E+07	1.47E+08	1.01E+08	1.82E+08
85	0.168	1	0.842	1	6.48E+06	7.36E+07	1.18E+07	3.92	1.61	90.91	6.5E+06	1.44E+08	2.62	0.04	97.34	7.4E+07	1.47E+08	1.01E+08	1.80E+08
86	0.16	0.95	0.85	1.01	6.10E+06	7.45E+07	1.12E+07	3.94	1.74	90.42	6.2E+06	1.46E+08	2.60	0.04	97.38	7.4E+07	1.47E+08	1.01E+08	1.80E+08
87	0.14	0.89	0.86	1.02	6.72E+06	7.53E+07	1.05E+07	3.94	1.86	89.74	5.8E+06	1.47E+08	2.57	0.04	97.39	7.5E+07	1.47E+08	1.02E+08	1.79E+08
88	0.13	0.82	0.87	1.03	6.31E+06	7.62E+07	9.74E+06	3.93	2.01	88.85	5.4E+06	1.48E+08	2.54	0.04	97.42	7.6E+07	1.47E+08	1.02E+08	1.78E+08
89	0.12	0.76	0.88	1.05	4.90E+06	7.71E+07	8.99E+06	3.90	2.17	88.03	5.0E+06	1.50E+08	2.51	0.04	97.45	7.7E+07	1.47E+08	1.03E+08	1.77E+08
90	0.11	0.70	0.89	1.05	4.49E+06	7.80E+07	8.24E+06	3.89	2.37	86.84	4.7E+06	1.52E+08	2.49	0.04	97.48	7.8E+07	1.47E+08	1.03E+08	1.76E+08
91	0.1	0.63	0.9	1.07	4.09E+06	7.89E+07	7.49E+06	3.87	2.61	86.53	4.3E+06	1.54E+08	2.45	0.04	97.51	7.9E+07	1.47E+08	1.03E+08	1.75E+08
92	0.09	0.57	0.91	1.08	3.68E+06	7.97E+07	6.74E+06	3.87	2.90	84.04	3.9E+06	1.55E+08	2.43	0.04	97.54	8.0E+07	1.47E+08	1.04E+08	1.74E+08
93	0.08	0.51	0.92	1.09	3.27E+06	8.06E+07	5.99E+06	3.86	3.26	82.04	3.5E+06	1.57E+08	2.40	0.03	97.56	8.0E+07	1.47E+08	1.04E+08	1.73E+08
94	0.07	0.44	0.93	1.10	2.86E+06	8.15E+07	5.24E+06	3.85	3.72	79.48	3.2E+06	1.59E+08	2.37	0.03	97.59	8.1E+07	1.47E+08	1.05E+08	1.72E+08
95	0.06	0.38	0.94	1.12	2.45E+06	8.24E+07	4.49E+06	3.85	4.35	76.06	2.9E+06	1.60E+08	2.35	0.03	97.62	8.2E+07	1.47E+08	1.05E+08	1.71E+08
96	0.05	0.32	0.95	1.13	2.04E+06	8.32E+07	3.75E+06	3.84	5.21	71.27	2.6E+06	1.62E+08	2.32	0.03	97.64	8.3E+07	1.47E+08	1.06E+08	1.70E+08
97	0.04	0.26	0.96	1.14	1.63E+06	8.41E+07	3.00E+06	3.84	6.52	64.06	2.0E+06	1.64E+08	2.30	0.03	97.67	8.4E+07	1.47E+08	1.06E+08	1.69E+08
98	0.03	0.19	0.97	1.15	1.23E+06	8.50E+07	2.25E+06	3.83	8.89	52.11	1.7E+06	1.65E+08	2.28	0.03	97.69	8.5E+07	1.47E+08	1.07E+08	1.68E+08
99	0.02	0.13																	