Department of Energy
Carlsbad Field Office
P. O. Box 3090
Carlsbad, New Mexico 88221

NOV 2 1 2006

Mr. Juan Reyes
U.S. Environmental Protection Agency
1200 Pennsylvania Avenue, NW
Washington, D.C. 20460

Subject: Uncertainty Analysis for the Planned Change Request on Magnesium Oxide (MgO) Emplacement

Dear Mr. Reyes:

This letter and its enclosures provide an uncertainty analysis that supports the U.S. Department of Energy's (DOE's) request for a reduction in the amount of magnesium oxide (MgO) emplaced at the Waste Isolation Pilot Plant (WIPP). The DOE currently emplaces 1.67 moles of MgO for every mole of organic carbon in cellulose, plastic, and rubber (CPR) materials that are emplaced in the WIPP. When the DOE requested that the MgO emplacement factor be reduced from 1.67 to 1.2 (letter Moody to Cotsworth, April 10, 2006), the EPA requested that the DOE address "the uncertainties related to MgO effectiveness, the size of the uncertainties, and the potential impact of the uncertainties on long-term performance" (letter Gitlin to Moody, April 28, 2006).

In response to the EPA's request, the DOE has analyzed the uncertainties associated with MgO. The enclosures to this letter document the results of the DOE's analyses. These enclosures are as follows:

- The *Overview of the MgO Uncertainty Analysis* is a brief, high-level summary of the key results from the uncertainty analysis and of the rationale for selecting an MgO emplacement factor of 1.2.
- The *Uncertainties Affecting MgO Effectiveness and Calculation of the MgO Effective Excess Factor* is the key technical report for the uncertainty analysis. It provides an integrated analysis for 15 types of uncertainty related to the effectiveness of MgO, and provides a quantitative assessment for the proposed MgO emplacement factor of 1.2.
- Four technical studies that evaluate specific aspects of repository response as they relate to the effectiveness of MgO. The technical studies evaluate: (i) the uncertainties related to carbonate precipitation, (ii) other uncertainties related to geochemistry, (iii) the amount of sulfate that could enter the repository from Castile brine and the amount of MgO that could be lost due to movement of that brine out of the repository, and (iv) the effectiveness of mixing processes in the repository.
- Two additional studies that evaluate the measurement uncertainty for CPR materials in the emplaced waste and the amount of reactive constituents in the bulk MgO supplied by Martin Marietta.

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These reports provide a comprehensive response to the EPA's request for an uncertainty analysis and to associated technical issues. If you have any questions regarding these reports, please contact Russell Patterson at (505) 234-7457.

Sincerely,

David C. Moody

David C. Moody
Manager

cc: w/enclosures
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OVERVIEW OF THE MgO UNCERTAINTY ANALYSIS

The U. S. Department of Energy (DOE) currently emplaces 1.67 moles of magnesium oxide (MgO) backfill for every mole of organic carbon in the cellulose, plastic, and rubber (CPR) materials that are emplaced in the Waste Isolation Pilot Plant (WIPP). The value of 1.67 represents a 67% excess over the amount of MgO that is required to react with the maximum amount of carbon dioxide that could be generated by microbial processes under conservative assumptions. The U. S. Environmental Protection Agency (EPA) has stated that this "relatively high excess amount" is required because "the extra MgO would overwhelm any perceived uncertainties that the chemical reactions would take place as expected" (Gitlin 2006). When the DOE requested that the MgO loading factor be lowered from 1.67 to 1.2, the EPA requested that the DOE address "the uncertainties related to MgO effectiveness, the size of the uncertainties, and the potential impact of the uncertainties on long-term performance" (Gitlin 2006).

The DOE's uncertainty analysis starts with a number of conservative assumptions: (i) microbes remain active through the lifetime of the repository, (ii) microbes will consume all of the organic carbon in the CPR materials that are emplaced in the repository, and (iii) other materials in the waste, such as lime and the corrosion products of iron-based materials, do not react with carbon dioxide (CO_2). The use of these assumptions maintains a conservative framework for determining the required amount of MgO in the repository.

The DOE evaluated 15 uncertainties related to MgO effectiveness, grouped into three categories:

1. Uncertainties in the quantities of CO_2 produced by microbial consumption of the organic carbon in the emplaced CPR materials
    a. Estimated amounts of CPR material in a room
    b. Effective yield of CO_2 per mole of emplaced organic carbon
    c. Role of methanogenesis

2. Uncertainties in the amount of MgO that is available to react with CO_2
    a. Fraction of reactive constituents in MgO
    b. Carbonation of MgO prior to emplacement
    c. Extent of reaction of MgO and/or brucite with CO_2
    d. Loss of MgO to brine outflow from the repository
    e. Likelihood of supersack rupture
    f. Amount of MgO in each room
    g. Efficiency of mixing processes
    h. Physical segregation of MgO from CO_2

3. Uncertainties in the moles of CO_2 sequestered per mole of MgO that is available to consume CO_2.
    a. Conversion of hydromagnesite to magnesite
    b. Consumption of CO2 by materials other than MgO
    c. Dissolution of CO_2 in WIPP brines
    d. Incorporation of CO_2 in biomass

Whenever possible, uncertainties were quantified and represented as random variables. The remaining uncertainties were reviewed qualitatively and are included via assumptions in the final estimation of MgO effectiveness. The results from the uncertainty analysis are dominated by Items 1b and 1c, the effective yield of CO_2 and the role of methanogenesis. These items are important because the yield of CO_2 per mole of organic carbon can be substantially less than previously assumed.

The uncertainty analysis for Items 1b and 1c has evaluated the yield of CO_2 per mole of organic carbon based on two microbial pathways: Pathway 1, when unlimited sulfate is always available from the waste and from natural sources, and Pathway 2, when sulfate is limited to that present in the emplaced waste. These two pathways represent the extremes in microbial gas generation because methanogenesis never occurs in Pathway 1 while it occurs to its maximum extent in Pathway 2. Further details on the pathways are provided in the report, *Uncertainties Affecting MgO Effectiveness and Calculation of the MgO Effective Excess Factor.*

For Pathway 1, enough sulfate enters the repository from the sulfate-bearing minerals and brine in the host rock to prevent methanogenesis; however, these minerals (anhydrite, gypsum, and polyhalite) also provide a natural source of calcium ions that can react with carbon dioxide, precipitating carbonate minerals. With precipitation of carbonate minerals, the uncertainty analysis demonstrates that the effective yield of CO_2 has a mean value of 0.72 moles of CO_2 per mole of organic carbon. For Pathway 2, methanogenesis consumes more than 94% of organic carbon in the waste and denitrification and sulfate reduction consume the remainder in the waste. Since methanogenesis produces 0.5 moles of CO_2 per mole of carbon and denitrification and sulfate reduction produce 1 mole of CO_2 per mole of carbon, the effective yield is given by 0.53 moles of CO_2 per mole of carbon in the waste. Thus, the effective yield of CO_2 lies within the narrow range of 0.53 to 0.72 moles of CO_2 per mole of organic carbon for the two pathways that represent the extremes of the microbial response.

The uncertainty analysis is based on an MgO loading factor of 1.2, consistent with the DOE's planned change request to the EPA. This loading factor implies a 20% excess of MgO if the effective yield is 1 mole of CO_2 per mole of organic carbon. However, this uncertainty analysis demonstrates that the excess amount of MgO is significantly greater than 20% because the expected yield of CO_2 is between 0.53 and 0.72. Conservatively taking the maximum value of the revised yield (0.72) into account, the full uncertainty analysis demonstrates that the mean or expected value of the effective loading factor is 1.6, or an excess MgO amount of 60%.

The uncertainty analysis also predicts a distribution for the effective loading factor, which defines the probability of having various excess amounts of MgO. The probability that the effective loading factor will be less than 1, the minimum amount of MgO required to sequester all CO_2, is of particular interest. The probability of an effective MgO loading factor less than 1 is calculated to be on the order of 10^{-19} for the distribution from this uncertainty analysis.

Given the conservative assumptions used in defining the 1.2 loading factor and the extremely small probability of a 1.2 loading factor not providing enough MgO to sequester all of the CO_2 generated, the uncertainty analysis provides confidence that an MgO loading factor of 1.2 defines a mass of MgO that will remain effective under all repository conditions.