

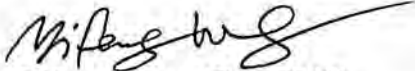
WPO 30743

Sandia National Laboratories

Albuquerque, New Mexico 87185-1341

date: May 9, 1996

to: Distribution



from: Yifeng Wang (Org. 6748)

subject: Evaluation of the Thermal Effect of MgO Hydration for the Long-Term WIPP Performance Assessment

The hydration reaction of backfill MgO with inflow brines can potentially change repository temperatures, due to the exothermic nature of the reaction. This memorandum is to evaluate the thermal effect of MgO hydration on the long-term WIPP performance assessment.

To simplify the problem, we assume that MgO hydration can be described by the overall reaction:



and that the reaction rate is much higher than the brine inflow rate and, therefore, the reaction will be limited by brine inflow. Considering the dimensions of the repository, we also assume that the heat released from the reaction will be dissipated away mainly from the ceiling and ground of the repository and the heat loss from the side walls is negligible. In addition, we assume that the hydration reaction will take place uniformly in a reaction region, which can be a panel or the whole repository.

Based on these assumptions, the thermal effect of MgO hydration can be modeled by a simplified system shown in Figure 1. The temperature distribution (T) can be described by the following equations:

$$C_p \rho \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial X^2} \quad (2)$$

$$T(X,0) = T_0 \quad (3)$$

$$\rho_w V \Delta H = -2Sk \left. \frac{\partial T}{\partial X} \right|_{x=0} \quad (4)$$

$$T(\infty, t) = T_0 \quad (5)$$

where C_p is the heat capacity of surrounding rocks; ρ is the molar density of surrounding rocks; t is time; X is the spatial coordinate; k is the thermal conductivity of surrounding rocks; T_0 is the background temperature; ρ_w is the molar density of water; V is the brine inflow rate; ΔH is the enthalpy change in Reaction (1); S is the horizontal area of the reaction region.

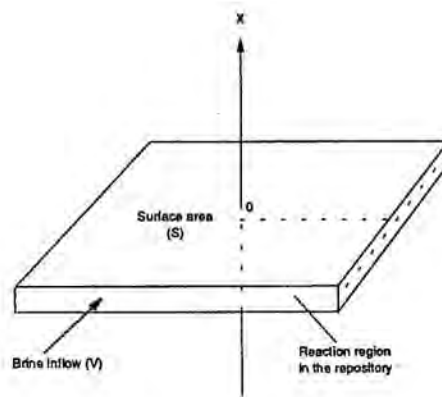


Figure 1. A modeling system for hydration heat production and heat conduction.

The above equations can be solved for T with a Laplace-transformation method:

$$T - T_0 = \frac{\rho_w V \Delta H}{2S \sqrt{C_p \rho k}} \left[2 \sqrt{\frac{t}{\pi}} e^{-\frac{C_p \rho X^2}{4kt}} - \sqrt{\frac{C_p \rho}{k}} X \operatorname{erfc} \left(\frac{X}{2} \sqrt{\frac{C_p \rho}{kt}} \right) \right]. \quad (6)$$

The temperature increase in the repository (ΔT) is obtained by setting $X = 0$ in equation (6):

$$\Delta T = T(0, t) - T_0 = \frac{\rho_w V \Delta H}{S} \sqrt{\frac{t}{\pi C_p \rho k}}. \quad (7)$$

Equation (7) shows that the repository temperature will increase with t until all MgO becomes hydrated. Therefore, the maximum temperature increase (ΔT_{\max}) in the repository can be calculated by

$$\Delta T_{\max} = T(0, t) - T_0 = \frac{\Delta H}{S} \sqrt{\frac{\rho_w V M_{\text{MgO}}}{\pi C_p \rho k}} \quad (8)$$

Where M_{MgO} is the inventory of MgO in the reaction region.

To be consistent with actinide solubility calculations, we assume that the reaction will occur uniformly in the whole repository, i.e., the reaction region shown in Figure 1 will extend to the whole repository. Then, $S = 1.1 \times 10^5 \text{ m}^2$ and $M_{\text{MgO}} = 2 \times 10^9 \text{ moles}$. The other parameters are estimated as follows:

$$\rho_w = 5.56 \times 10^4 \text{ moles/m}^3;$$

Information Only

maximum $V = 1000 \text{ m}^3/\text{year}$ (Joel Miller, personal communication);

$\Delta H = 3.89 \times 10^4 \text{ J/mole}$ (Drever, 1982);

$\rho = 3.7 \times 10^4 \text{ moles/m}^3$ (Lide, 1994), assuming that the surrounding rocks can be represented by halite;

$C_p = 50 \text{ J/mole/K}$ (Lide, 1994), assuming that the surrounding rocks can be represented by halite;

$k = 6.3 \text{ W/m/K} = 1.99 \times 10^8 \text{ J/year/m/K}$ (Lide, 1994), assuming the surrounding rocks can be represented by halite.

From these data, we estimate the maximum temperature increase in the repository due to MgO hydration to be 3.4 K. Therefore, the thermal effect of MgO hydration can be negligible.

References:

- Drever J. I. (1982) The Geochemistry of Natural Water. Prentice-Hall.
Lide D. R. (1994) Handbook of Chemistry and Physics. CRC Press.

Distribution:

- MS 1320 J. Nowak (Org. 6831)
- MS 1320 R. V. Bynum (Org. 6831)
- MS 1328 C. T. Stockman (Org. 6749)
- MS 1335 M. S. Y. Chu (Org. 6801)
- MS 1341 C. C. Crafts (Org. 6748)
- MS 1341 J. T. Holmes (Org. 6748)
- MS 1341 B. M. Butcher (Org. 6748)
- MS 1341 L. H. Brush (Org. 6748)
- MS 1341 Y. Wang (Org. 6748)
- MS 1341 R. F. Weiner (Org. 6751)
- MS 1343 A. S. Reiser (Org. 6751)
- MS 1330 SWCF-A (Org. 6352), WBS.1.1.09.1.1(RC)

Information Only