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U.S. Nuclear Regulatory Commission  
ATTN: Mrs. Deborah A. DeMarco  
Office of Nuclear Material Safety and Safeguards  
Program Management, Policy Development, and Staff  
Office of the Director  
Mail Stop 8D-37  
Washington, DC 20555

Subject: Programmatic Review of Abstracts

Dear Mrs. DeMarco:

The enclosed abstracts are being submitted for programmatic review. These abstract will be submitted for presentation at the Goldschmidt 2002 Conference, to be held August 18-23, 2003, in Davos, Switzerland. The title of these abstracts are:

"Effects of Salt Formation on the Chemical Environment of a High-Level Nuclear Waste Repository" by R.T. Pabalan, L. Yang, and L. Browning

"Computer Simulation of Uranyl Adsorption on Montmorillonite Clay" by O.F. Zaidan, J.A. Greathouse, and R.T. Pabalan

These abstracts are a product of the CNWRA and do not necessarily reflect the view(s) or regulatory position of the NRC.

Please advise me of the results of your programmatic review. Your cooperation in this matter is appreciated.

Sincerely,



Budhi Sagar  
Technical Director

BS: ar

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## Enclosures

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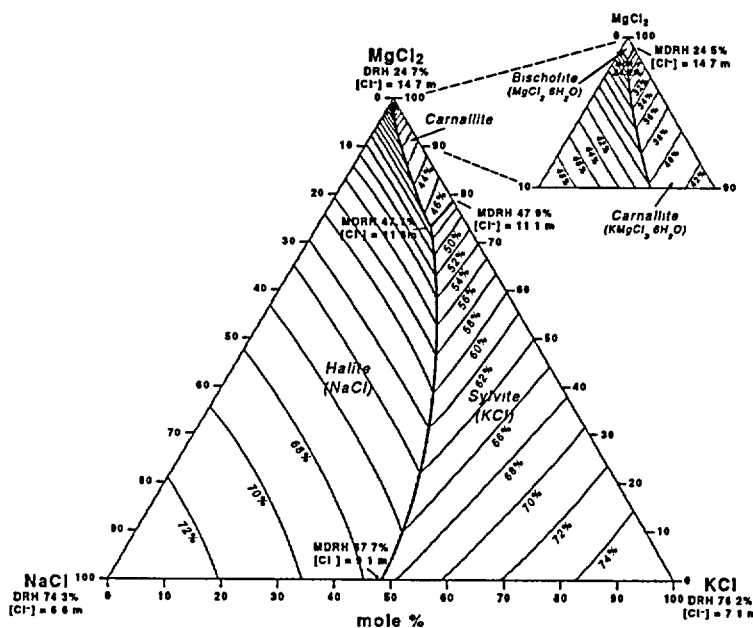
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# Effects of Salt Formation on the Chemical Environment of a High-Level Nuclear Waste Repository

R. T. PABALAN, L. YANG, AND L. BROWNING

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In the absence of mechanical disruption, aqueous corrosion will be the primary degradation process limiting the life of waste packages (WPs) and drip shields (DSs) in the proposed high-level nuclear waste repository at Yucca Mountain (YM), Nevada. In a hot repository setting, evaporation processes would increase the aqueous concentrations of  $\text{Cl}^-$ ,  $\text{F}^-$ , and other ions and lead to the accumulation of multicomponent salt deposits on DS and WP surfaces. Inorganic salts are generally hygroscopic and will absorb moisture from humid air, generating small volumes of potentially corrosive brines. In this study, thermodynamic modeling was done to evaluate the effect of salt formation on the chemical environment of DSs and WPs at the proposed repository. The deliquescence behavior of salt mixtures was calculated using thermodynamic considerations and compared with that of single salts. Also, the chemical evolution of YM porewaters was evaluated to determine the types of brines and salt mixtures that could form by evaporation processes. The results are consistent with published data that show the deliquescence points of salt mixtures are lower than those of individual salts (Figure 1). Mixtures containing Mg and Ca salts have much lower deliquescence points than pure  $\text{NaNO}_3$ , which is used by the U.S. Department of Energy (DOE) to bound the deliquescence point of salt mixtures. Formation of Mg and Ca salts could lead to earlier initiation of aqueous corrosion than assumed by the DOE in its performance assessment modeling. Such mixtures can be formed by evaporation of waters with compositions similar to some Yucca Mountain porewaters.



**Figure 1.** Calculated mutual deliquescence relative humidity, MDRH (%) [contour lines] of salt mixtures in the system NaCl-KCl-MgCl<sub>2</sub> at 90 °C. The solutions are saturated with the indicated solids.

## **Acknowledgment**

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## Computer Simulation of Uranyl Adsorption on Montmorillonite Clay

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### Introduction and Methods

We have performed Monte Carlo computer simulations to study the adsorption characteristics of the aqueous uranyl ion ( $\text{UO}_2^{2+}$ ) near the basal plane of montmorillonite, a smectite clay. The aim of this research is to better understand the fate of uranium waste products in groundwater and their retention by soil sediments, a problem of increasing importance in environmental geochemistry.

Details of our simulation technique and potential parameters for montmorillonite are reported elsewhere (Skipper et al., 1995). Potential parameters for the uranyl ion yield a coordination geometry consistent with x-ray diffraction data (Gilbaud et al., 1996).

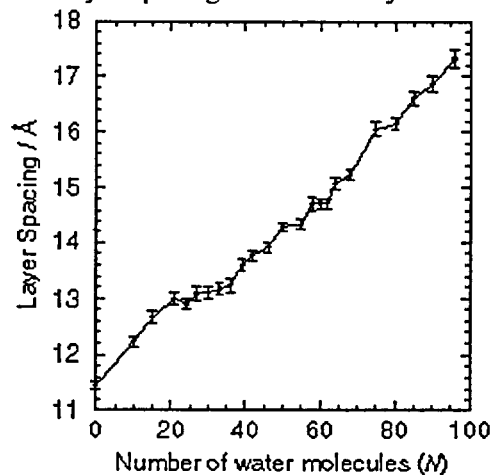
### Results

Figure 1 shows the  $d(001)$  profile as the interlayer water content ( $N$ ) is increased from 0 to 96 (300 mg  $\text{H}_2\text{O}$  / g clay). A stable swelling state is seen at 14.7 Å at  $N = 55-60$ . This value agrees well with the experimental values of 14.81 Å (Giaquinta et al., 1997). The simulation also shows that each uranyl ion is coordinated by 5 water molecules and is oriented with the O-U-O axis tilted slightly off parallel to the clay's basal plane.

### Acknowledgment

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Figure 1: Layer spacing versus interlayer water content.



## References

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- Skipper N.T., Chang F.-R.C. and Sposito G., (1995), *Clays Clay Miner.* 43, 285-293.