

TRIP REPORT

SUBJECT: Near Field Performance Assessment Workshop

DATE AND PLACE: October 15-17, 1990  
Madrid, Spain

AUTHOR: William M. Murphy

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### TRIP REPORT

**SUBJECT:** Near Field Performance Assessment Workshop  
**DATE and PLACE:** October 15-17, 1990; Madrid, Spain  
**AUTHOR:** William M. Murphy  
**PERSONS PRESENT:** Participant list is enclosed in Appendix 2.

#### BACKGROUND AND PURPOSE:

The stated purpose of the workshop organized by ENRESA, the Spanish nuclear waste agency, and sanctioned by the Commission of European Communities, was to "review and compare approaches of near-field performance assessment for high-level waste disposal." William Murphy was invited by the conference organizers to make a technical presentation on the near-field environment.

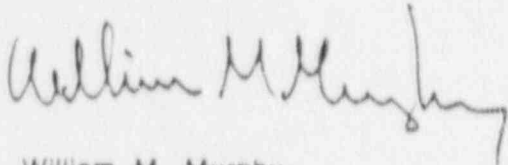
#### SUMMARY AND CONCLUSIONS:

The schedule of presentations is attached in Appendix 2. Proceedings of the workshop will be published by SKB, the Swedish nuclear waste agency. The meeting started with brief descriptions of international high-level waste (HLW) programs. These were followed by the presentation on the near-field environment, and by presentations on other aspects of near-field performance assessment (NFPA). Summaries of the talks are given in Appendix 1. Abundant time for group discussions was scheduled, and interactions were generally lively among a subset of participants. Other individuals, notably a USDOE representative with administrative responsibility, appeared to sleep through most of the meeting. This *ad hoc* meeting gathered experts in a field that currently has no specific regular forum for exchange. The benefit of establishing a permanent or regular working group was debated, and will be pursued by the primary organizers, Mick Apted (formerly of Pacific Northwest Laboratory), Patrick Sellin (of SKB), and Jose Gago (of ENRESA). An international forum on NFPA would be useful because of the numerous components (*e.g.* waste forms, containers, packing) and processes (*e.g.* thermal-hydrological-mechanical-chemical perturbations/coupling, solubilities, redox relations, radiolysis) are common to many programs. Particularly, solubility studies would benefit from international collaboration because of the tedium of the work.

Benchmarking and validation of "near-field performance assessment codes" appear to be premature based on the apparent state of the art, and may be unrealistic in general. General understanding and resources and computing ability should permit development of highly site specific NFPA codes, rather than a generic NFPA code that could be used at many sites. One would not expect comparable (benchmarkable) results from them. The strict concept of validation (comparison of model with empirical results) appears to be inappropriate to performance assessments. Nevertheless, detailed subsystem models should be validated, and NFPA models need to be examined and justified and supported by confirming studies (*e.g.* natural analogs). The purpose of a PA model is not to reproduce empirical results or even to predict the real evolution of a

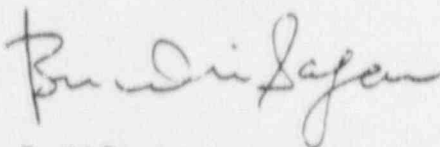
set of processes in a repository. In general PA models deliberately deviate from reality in attempting to be conservative in their assessments. There are many ways to be conservative; one would not expect each code to use the same approach; and one would not expect different codes to produce the same results or to be strictly comparable.

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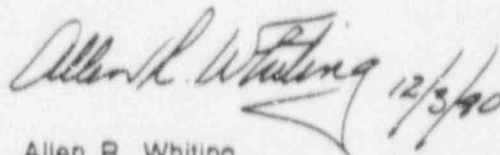


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Senior Research Scientist

**CONCURRENCE SIGNATURES AND DATES**



Budhi Sagar  
Manager - Performance Assessment



Allen R. Whiting  
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**Appendix 1. Summary of Presentations.**

**Murphy:** Post-emplacment environment. Thermal, hydrologic, mechanical, and chemical effects relevant to performance assessment in the near-field environment were described generally and illustrated by the results of detailed analyses related to the proposed Yucca Mountain repository. The manuscript to be published for this presentation has been reviewed at the CNWRA and will undergo NRC programmatic review.

**Grogan:** Benchmarking. The concept of benchmarking performance assessment codes was presented generally to consist of the following components: Comparison of conceptual models; realistic test problems; parameter sensitivity studies; and comparisons of the results of computations with different codes.

**Grambow:** Glass release. Short-term dissolution rates are controlled by diffusion, long-term rates by matrix dissolution and solubility effects. Results by Jantzen and Plodinec (1983) and Pederson et al. (1983) showed the dependence of the rate on the free energy of reaction. The free energy may not correspond to the overall reaction but to silica release only (e.g. Bourcier, 1989). Surface layers or secondary phases can control the silica concentration and the rate of release. Van Iseghem et al. (1990) showed that the release rate can increase with the inception of zeolite formation. Silica adsorption on iron oxides can increase dissolution rates.

Garisto: Spent-fuel release. Release from the gap and leaching from grain boundaries is rapid (modeled as instantaneous), dissolution of grains is slow. Metallic alloys in grain boundaries contain significant Tc. Oxidation to  $U_3O_8$  must occur by dissolution-precipitation and results in loss of radionuclides. Oxidation rate may increase with the carbonate content of water. If all  $\alpha$  radiolysis leads to dissolution then high rates result. If the near-field is reducing then  $\alpha$  radiolysis leads only to  $U_4O_7$ , structural reorganization of the spent fuel does not occur, and radionuclides are not released.

Nitsche: Solubility. Criteria for valid solubility studies are: demonstrated equilibrium; effective separation of solid and solution; well defined solid phase; knowledge of speciation/oxidation state of solution. Americium precipitation experiments limits solubilities to about  $1 \times 10^{-10}$  M. Self  $\alpha$  radiation can decrease crystallinity and increase solubility. Pu(V) forms dominant aqueous species in oxidizing solutions. Pu(IV) carbonates have decreasing solubility with increasing temperature. Np(V) solubility decreases with pH forming Na-Np carbonates. Solubility studies relevant to Yucca Mountain (e.g. oxidizing carbonate environment) appear to be limited to simple phases.

Neretneiks: Near-field transport processes. Transport through bentonite packing is by diffusion. Advection in fractures in rock can be important. Fractures are heterogeneous and very localized. Results of performance assessments can be improved by taking account of slow transport through barriers such as corroded containers.

McKinley: Integrated near-field assessment. Models of the performance of repositories are generally extremely conservative; real repositories would perform much better. Two essential features of geologic repository sites are low fluid fluxes and a chemically reducing environment. The 1 part in  $10^5$  release requirement of the NRC is unrealistic. Geosphere requirements are not great if the near field is tight.

Jamet: Coupled processes. Two types of coupled processes are: *Sensu-stricto* (e.g. cross term effects of gradients in physical phenomena); and hidden (e.g. transport and geochemistry, flow and temperature, stress and temperature, fluid path and mineral precipitation). *Sensu-stricto* effects were discussed theoretically. An example was given showing that the Soret effect in a hypothetical near-field environment can multiply fluxes by 3 or 4 times in a high thermal gradient.

Umeki: Sensitivity Analyses and Validation.

Apted: Future directions and needs. A potpourri of issues was addressed, with an emphasis on the overriding significance of the near-field in performance assessment.

## MONDAY, OCTOBER 15

9:00-9:45	Coffee/ Introductions by Organizing Committee (Informal)	
9:45-10:00	Opening of Workshop Welcoming Address by ENRESA	Gago/ Spain Ulibarr/ Spain
10:00-11:00	Technical Presentations on National HLW Programs for Near-Field Performance Assessment Sweden - P. Sellin/ SKB Canada - L. Johnson/ AECL Belgium - G. Volckaert/ CEN/SCK Japan - S. Masuda/ PNC France - S. Voinis/ CEA	Gago/ Spain
11:00-11:30	Break	
11:30-13:00	Technical Presentations on National Programs (cont) Switzerland - I. McKinley/ Nagra Finland - T. Vieno/ VTT Spain - J. Grávalos/ ENRESA United States - R. Levich/ USDOE Germany - R. Storck/ Institut für Tieflagerung Korea - Kyong Won Han/ KAERI United Kingdom - R. G. G. Holmes/ BNF Taiwan - Shang-Jyh Liu/ INER NEA - H. Wanner/ NEA	Sellin/ Sweden
13:00-15:50	INDEPENDENT ACTIVITIES	
15:50-16:00	Introduction to Technical Sessions	Apted/ USA
16:00-16:45	INVITED TALK "Post-Emplacement Environment"	Murphy/ USA
16:45-17:30	Open Discussion	Sharland/ UK
17:30-18:00	INVITED TALK "Benchmarking"	Grogan/ UK
18:00-18:30	Open Discussion	Johnson/ Canada
18:30	END OF FIRST DAY	

## WEDNESDAY, OCTOBER 17

9:00-9:30	INVITED TALK "Integrated Near-Field Assessment"	McKinley/ Switzerland
9:30-10:15	Open Discussion	Voinis/ France
10:15-10:45	INVITED TALK "Sensitivity Analyses and Validation"	Umeki/ Japan
10:45-11:30	Open Discussion	McGrail/ USA
11:30-11:45	Break	
11:45-12:30	INVITED TALK "Future Directions and Needs"	Apted/ USA
12:30-14:00	Open Discussion	Sellin/ Sweden
14:00-14:10	Closing Remarks	Gago/ Spain
14:10	END OF WORKSHOP	
14:10-16:30	<i>Meeting on Proceedings Volume</i>	<i>Speakers and Discussion Leaders</i>

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