

OAK RIDGE NATIONAL LABORATORY

OPERATED BY MARTIN MARIETTA ENERGY SYSTEMS, INC.

POST OFFICE BOX X  
OAK RIDGE, TENNESSEE 37831

August 28, 1984

WM BUCKET CONTROL  
CENTER

SEP 10 P. 10  
'84

Dr. W. Dam  
Geotechnical Branch  
Office of Nuclear Materials  
Safety and Safeguards  
U.S. Nuclear Regulatory Commission  
Willste Building  
Washington, DC 20555

WM-RES  
WM Record File  
B-0287  
ORNL

WM Project 10, 11, 16  
Docket No. \_\_\_\_\_

PDR ✓  
LPDR B, N, S

Distribution:

DAM  
BROOKS  
(Return to WM, 623-SS) ✓

CC: STARMER

Dear Bill:

While at the ONWI geochemistry program overview, I spoke with John Starmer about the introductory statements which the NRC and I need to prepare for the workshop on geochemical modeling. John suggested I discuss the content of the remarks with you. I have prepared a preliminary outline for the introductory section and included suggestions for the NRC portion of the introduction. Please look these over and let me know what you think is appropriate. The NRC representative will have approximately 10 - 12 minutes to speak. Part of my selection of material is based on my assumption that the NRC already has some existing slides/vu-graphs which portray the necessary relationships.

Welcome and Introduction: Gary K. Jacobs

Regulatory Framework: NRC Representative

- A) Regulatory Framework: 3 - 4 slides explaining the NRC, EPA, and DOE regulations.
- B) NWPA schedule.
- C) What is a repository: 3 - 4 slides illustrating the definitions of geologic setting, disturbed zone, waste package, accessible environment, etc.
- D) Definitions: performance assessment, site characterization, etc. - what they are and how they will be used.

Summary of Issues: Gary K. Jacobs

My introductory comments in this section will focus specifically on geochemical models - what they are and possible applications. I also will briefly summarize the list of issues to be addressed during the workshop and the goals of the workshop as stated in the original announcement for the workshop.

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August 28, 1984

As time is getting short I would appreciate your looking over these suggestions and getting back to me as quickly as possible. If you have any questions please call me at (FTS) 626-0567.

Sincerely,



Gary K. Jacobs

GKJ:kk

Enclosures: list of issues  
workshop announcement

cc: R. J. Starmer, Geochemistry Section, Geotechnical Branch, NRC  
S. K. Whatley  
GKJ-File

Issues Concerning  
The Application of Geochemical Models to High-Level  
Nuclear Waste Repository Assessment

Issue #1:

*What role(s) should geochemical modeling play in characterizing and understanding the nature and performance of high-level radioactive waste repositories?*

Specifically, what are the capabilities and limitations of geochemical models in:

- A) Elucidating the nature of, and the controls on, geochemical conditions in the undisturbed geologic setting. Important variables for consideration include: temperature, pressure, groundwater chemistry, pH, redox potential, mineralogy of host rocks, etc.
- B) Evaluating effects within the disturbed zone. Important considerations include: physicochemical interactions between heated groundwater, host rocks, and engineered materials; radiation damage to solids and radiolysis of groundwaters; residual effects of repository construction, etc.
- C) Quantifying the release and transport of radionuclides from the waste packages through the disturbed zone and geologic setting to the accessible environment. Applications of geochemical models to this activity could include: (1) predictive performance assessment modeling of the release and transport of radionuclides, and (2) evaluation of experimental data from solubility and sorption tests.

Issue # 2:

*What are some of the key developments (forthcoming and long-term goals) which could enhance the role of geochemical modeling in repository assessments?*

Specific areas of consideration would include:

- A) Theory and Code Development. For example, which of the following topics, if any, represent important development areas for the successful application of geochemical models to repository assessments: (1) high ionic strength solution theory, (2) kinetic processes, (3) theoretical sorption calculations, (4) uncertainty analysis, and (5) data base and code verification, documentation, and management.
- B) Coupled Processes. For example, to what extent would the coupling of one or more thermodynamic, kinetic, and fluid flow processes be useful and appropriate for repository assessments?
- C) Data Needs. For example, which thermodynamic and kinetic data need to be obtained to increase the applicability of geochemical models to high-level nuclear waste repository systems. Which experimental and field validation studies could best increase the level of confidence in assessments utilizing geochemical models?

## **PRELIMINARY PROGRAM**

### **Workshop on the Application of Geochemical Models to High-Level Nuclear Waste Repository Assessment**

**October 2-5, 1984**

**Pollard Auditorium  
Oak Ridge Associated Universities  
Oak Ridge, Tennessee**

**Sponsored by: U.S. Nuclear Regulatory Commission  
and  
Oak Ridge National Laboratory**

#### **Tuesday morning, October 2**

**10:30 Coffee and Registration**

#### **Tuesday afternoon, October 2**

**1:00 Welcome and Introduction—G. K. Jacobs, Oak Ridge National Laboratory, Oak Ridge, Tennessee; R. J. Starmer, Nuclear Regulatory Commission, Washington, D.C.**

#### **Session I. Solution Chemistry: Theory, Code Development, Non-Repository Applications**

**Chairman: H. L. Barnes, Pennsylvania State University,  
University Park**

**1:30 Thermodynamic Problems in Speciation Modeling—H. L. Barnes, Pennsylvania State University, University Park**

**2:15 Prediction of Mineral Solubilities in High-Temperature and High-Ionic-Strength Solutions—J. H. Weare, University of California, San Diego**

**3:00 Intermission**

**3:15 Summary and Discussion—Panel and Participants**

**4:15 Announcements and Adjournment**

**Wednesday morning, October 3**

**Session I. Solution Chemistry: Theory, Code Development,  
Non-Repository Applications**

**Chairman: H. L. Barnes, Pennsylvania State University,  
University Park**

- 8:30 PHREEQE: Status and Applications—**L. N. Plummer**, U.S. Geological Survey, Reston, Virginia
- 9:15 MINTEQ: Status and Applications—**J. R. Morrey** and **K. M. Krupka**, Pacific Northwest Laboratory, Richland, Washington
- 10:00 Intermission
- 10:15 EQ3/EQ6: Status and Applications—**T. J. Wolery**, Lawrence Livermore National Laboratory, Livermore, California
- 11:00 Summary and Discussion—Panel and Participants
- 12:00 Lunch

**Wednesday afternoon, October 3**

**Session II. Data Base Development**

**Chairman: E. A. Jenne, Pacific Northwest Laboratory,  
Richland, Washington**

- 1:00 Thermodynamic Data for Geochemical Modeling for a High-Level Nuclear Waste Repository—**E. A. Jenne**, Pacific Northwest Laboratory, Richland, Washington
- 1:30 Complexes of Actinides with Naturally Occurring Organic Compounds—**G. R. Choppin**, Florida State University, Tallahassee
- 2:00 Experimental Determination of Stability Constants of the Carbonate Complexes of Uranium and Neptunium—**Leon Maya**, Oak Ridge National Laboratory, Oak Ridge, Tennessee
- 2:30 Intermission
- 2:45 Temperature Dependence of Actinide Solubilities and Speciation—**R. J. Silva**, Lawrence Berkeley Laboratory, Berkeley, California
- 3:15 Neptunium and Technetium Behavior in Geologic Systems—**R. E. Meyer**, Oak Ridge National Laboratory, Oak Ridge, Tennessee
- 3:45 Thermodynamic Properties of Geologic Materials: Status and Future—**J. L. Haas**, U.S. Geological Survey, Reston, Virginia
- 4:15 Summary and Discussion—Panel and Participants
- 5:00 Announcements and Adjournment

**Thursday morning, October 4**

**Session III. Coupled Processes: Thermodynamic, Kinetic, and Transport**

Chairman: F. J. Pearson, Jr., Intera Environmental Consultants,  
Houston, Texas

- 8:30 Mathematical Reaction-Transport Modeling of Nonequilibrium Water/Rock Interactions—**P. Ortoleva**, Indiana University and Geochem Research Associates, Inc., Bloomington, Indiana
- 9:15 Coupled Geochemical and Fluid-Flow Code Development—**J. R. Morrey**, Pacific Northwest Laboratory, Richland, Washington
- 9:45 Intermission
- 10:00 Comparison of Dissolution Versus Precipitation Kinetics in Silicates—**A. C. Lasaga**, Pennsylvania State University, University Park
- 10:30 Modeling of Reaction Processes and Fluid Flow in Complex Systems—**C. H. Moore**, Geochem Research Associates, Bloomington, Indiana
- 11:00 Summary and Discussion—Panel and Participants
- 12:00 Lunch

**Thursday afternoon, October 4**

**Session IV. Repository Applications of Geochemical Models**

Chairman: G. E. Grisak, Geologic Testing Consultants, Ltd.,  
Ottawa, Ontario, Canada

- 1:00 Canadian Program—**N. C. Garisto**, Atomic Energy of Canada, Ltd., Pinawa, Manitoba, Canada
- 1:30 Basalt Waste Isolation Program—**T. O. Early** and **C. F. McLane**, Rockwell Hanford Operations, Richland, Washington
- 2:00 Nevada Nuclear Waste Storage Investigation Program—**TBD**, Lawrence Livermore National Laboratory, Livermore, California, and **TBD**, Los Alamos Scientific Laboratory, Los Alamos, New Mexico
- 2:30 Intermission
- 2:45 Office of Crystalline Rock Development Program—**E. S. Patera**, Department of Energy, Chicago Operations Office, Argonne, Illinois
- 3:15 Office of Nuclear Waste Isolation Program—**J. B. Moody**, Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio
- 3:45 Summary and Discussion—Panel and Participants
- 4:00 Announcements and Adjournment

**Friday morning, October 5**

**8:30-12:30**

**Session V. Summary and Conclusions**

**Chairman: G. K. Jacobs, Oak Ridge National Laboratory  
Oak Ridge, Tennessee**

This session will include brief summary statements by each panel member concerning his/her respective session. The floor will then be opened for discussion (arranged according to session order) for each of the key topics and issues that were prepared prior to the workshop. Approximately 45 minutes of discussion will be allowed for each session topic. At the end of the discussion, a consensus statement will be developed by the pertinent member of the panel. Unless opposition remains on the floor, this statement will be taken to be a conclusion of the workshop. If extreme opposition should continue, then a compromise statement will be prepared, or both positions will be duly recorded.

**12:30 Closing Comments and Adjournment**

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**Program Committee**

G. K. Jacobs  
S. K. Whatley  
J. G. Blencoe  
A. D. Kelmers  
Oak Ridge National Laboratory

H. L. Barnes	Pennsylvania State University
G. E. Grisak	Geologic Testing Consultants, Ltd.
G. K. Jacobs	Oak Ridge National Laboratory
E. A. Jenne	Pacific Northwest Laboratory
F. J. Pearson, Jr.	Intera Environmental Consultants

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# **WORKSHOP ON THE APPLICATION OF GEOCHEMICAL MODELS TO HIGH-LEVEL NUCLEAR WASTE REPOSITORY ASSESSMENT**

**October 2-5, 1984**

**Oak Ridge, Tennessee**

Geochemical models and computer codes (e.g. solubility/speciation, reaction path, hydrothermal chemistry, etc.) may play an important role in helping to show reasonable assurance that high-level nuclear waste repositories can achieve the technical criteria and performance objectives set forth in current regulations. To meet this challenge a workshop is being sponsored by the U.S. Nuclear Regulatory Commission and Oak Ridge National Laboratory to discuss these calculational methodologies and their possible role in repository assessments. The purpose of the workshop is to summarize and discuss the current status of geochemical code development, data bases, reaction kinetics, coupled process models, and the application of geochemical models to high-level nuclear waste repository site characterization and performance assessment activities. The goal of the workshop is to develop a consensus, to the extent possible, on the capabilities and limitations of geochemical models for licensing activities related to high-level nuclear waste repositories.

The intent of the workshop is to bring together experts with diverse backgrounds in a structured forum to discuss the important topics related to geochemical models. In order to keep the size of the workshop to a manageable level, all speakers and attendees are by invitation or approved requests only. The sessions of the workshop will be chaired by a panel composed of the following members who have expertise in areas important to geochemical modeling and repository analysis:

H. L. Barnes	Pennsylvania State University
G. E. Grisak	Geologic Testing Consultants, Ltd.
G. K. Jacobs	Oak Ridge National Laboratory
E. A. Jenne	Pacific Northwest Laboratory
F. J. Pearson, Jr.	Intera Environmental Consultants

A workshop proceedings will be published and will be available to the technical community and public through the National Technical Information Service. The proceedings will contain extended abstracts of the presentations, summaries of the individual working sessions, and a discussion of recommendations. Papers, copies of visual aids, and transcripts of the presentations and discussions will not be included in order to promote the free exchange of the latest information available from each speaker; speakers are encouraged to bring handout materials for distribution at the workshop.



The workshop will consist of several sessions, each devoted to a particular topic. Interchange among speakers and participants during presentations will be encouraged, and ample time for discussion will be provided during and after each presentation and at the end of each session. Participants are encouraged to bring slides and/or vugraphs to facilitate any comments or rebuttals they may wish to make during the discussion periods. A list of discussion subjects and goals for the workshop will be distributed prior to the workshop. This list of issues will provide a means of focusing on the key topics during the workshop and will be used in developing a consensus from the workshop. The topics of the working sessions include:

- I. Solution Chemistry ... Theory, Code Development, Non-Repository Applications
- II. Data Base Development
- III. Coupled Processes: Thermodynamic, Kinetic, and Transport
- IV. Repository Applications
- V. Summary and Discussion

Additional information (including a list of discussion items) will be sent to you following acceptance of the invitation to the workshop. For additional information, please contact G. K. Jacobs [FTS telephone 626-0567, commercial telephone (615)-576-0567] or S. K. Whatley [FTS telephone 624-6135, commercial telephone (615)-576-6135].

Arrangements:

- When: October 2-5, 1984
- Location: Pollard Auditorium  
Oak Ridge Associated Universities  
Oak Ridge, Tennessee 37830
- Lodging: A block of rooms has been reserved at the Holiday Inn of Oak Ridge. Please make your arrangements through the Holiday Inn (615-483-4371).
- Registration: Registration will begin during the coffee period on Tuesday, October 2, at 10:30 AM at the Pollard Auditorium. A registration fee of \$65.00 is requested to cover miscellaneous costs and the dinner and entertainment on Tuesday. If you plan to attend the workshop, please fill out the attached registration form and send it with the registration fee by August 15 to:

S. K. Whatley  
Oak Ridge National Laboratory  
P.O. Box X  
Oak Ridge, Tennessee 37831

**Social Events:** A barbecue with blue-grass music is being planned for Tuesday evening at the Museum of Appalachia, Norris, Tennessee. The social hour starts at 6 PM with dinner to follow.

**Travel:** The McGhee-Tyson Airport of Knoxville is approximately 45 minutes from Oak Ridge and has frequent flights to and from Washington, DC, Atlanta, Denver, and other major U.S. cities. Local Oak Ridge-Knoxville route maps are enclosed for your convenience.

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**Pre-registration  
Workshop on  
Application of Geochemical Models to High-Level Nuclear Waste  
Repository Assessment**

**October 2-5, 1984**

**Oak Ridge, Tennessee**

(please print)

Name \_\_\_\_\_  
(last) (first) (middle initial)

Affiliation \_\_\_\_\_

Mailing Address \_\_\_\_\_

\_\_\_\_\_ Phone \_\_\_\_\_

**Registration Fee**

Entire Workshop (covers all sessions, Proceedings, social events, and intermission refreshments) \$65.00

Make check payable to:  
Oak Ridge National Laboratory

**TOTAL ENCLOSED \$**\_\_\_\_\_

The registration fee will be returned upon cancellation of registration prior to September 24, 1984.

Mail check and this card to:  
S. K. Whatley  
Oak Ridge National Laboratory  
P.O. Box X  
Oak Ridge, Tennessee 37831