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WM Record File

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WM Project

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Docket No.

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(Return to WM, 623-SS) Linehan w/ encl. July 29, 1985

See Packet 5 for encl.

MEMORANDUM FOR: Robert E. Browning, Director
Division of Waste Management

FROM: Paul T. Prestholt, Sr. OR-NNWSI

PYP

Subject: NNWSI Site Report for Weeks of July 1, 8, 15, & 22, 1985

I. On July 2, I had lunch with Don Vieth. We particularly discussed the USGS issue. Dallas Peck of the GS sent a letter to Ben Rusche outlining the GS position on implementing the USGS-DOE M.O.U. A copy of this letter is enclosed. I gathered that the GS position was not satisfactory to Dr. Vieth. Negotiations will continue until a workable solution is achieved. Dr. Vieth and his staff fully understand that an early solution is vital in keeping a reasonable schedule to licensing.

II. A QA audit of Lawrence Livermore National Laboratory was scheduled for the week of July 8. I attended as an observer. The LLNL Quality Assurance Program Plan was submitted to the NNWSI Quality Assurance Program Manager in accordance with procedures outlined in the NNWSI Quality Assurance Plan - NVD-196-17, Rev.3. Eighteen of 22 procedures of the LLNL QAP were reviewed and approved prior to the audit date. However, the approval of the 18 procedures was not received by LLNL until the day before the audit began.

During the first day of the audit (July 9) it became obvious to the audit team that LLNL had not had time to implement the newly approved procedures. Since the audit team was prepared to audit only procedure implementation and not the on-going work, the audit was postponed for 90 days.

It is my understanding that future audits will be on work being performed under whatever procedures are in force or that have been implemented at the time of the audit.

Only three of the nine organizations that are required to submit QAP's for approval under provisions of NVD-196-17, Rev.3 have been given approval of their procedures. These are LLNL,

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Westinghouse, and SAIC. Of the other 6, several are in review and the others have not yet been submitted. For instance, the USGS QAP's are in internal review and have not been submitted and LANL is still writing their procedures.

III. DOE-WMPO scheduled a tectonics workshop on July 22-23, with the USGS, SAIC, and Bechtel. The USGS included experts in specific technical areas. These experts are not part of the NNWSI program. An attendance list is included. Since I was invited to this meeting, it was decided that I would attend and skip the workshop held at LLNL. This decision also allowed me to attend the July PM-TPO meeting, held on the 24th & 25th.

The purpose of the tectonics workshop was to develop the tectonic scenarios to be used by the "Tectonic Position Paper Working Group" to flesh out the DOE tectonic position paper. The first day of the workshop was not very successful. The USGS experts used too much time trying to answer the suggested scenarios, in editorializing, and in expressing personal prejudices.

The session on the second day was attended by the working group and a few advisors; more was accomplished. A group of possible scenarios were identified and a draft technical position will be written for USGS concurrence.

A set of definitions were drafted by Bechtel National, Inc. for the Seismic/Tectonic Position Paper. These definitions, in draft, were presented to the working group for review and comment. A copy of the definitions is enclosed. I will forward, to the working group, any comment the NRC technical staff might want to make on the definitions.

The URS/John A. Blume organization prepared and proposed an outline for a NNWSI Seismic/Tectonic Position Paper. This is only a suggested outline for information only.

IV. The July TPO meeting was held on July 24 & 25. The following are items of interest to the staff:

1. WMPO now has a "Systems and Project Control" branch. Wendy Dixon has been appointed branch chief;
2. Joe Delugos has joined the WMPO geotechnical branch as a hydrologist;
3. Larry Ramspott, LLNL TPO, reported that the first day of the Waste Package Workshop went well;
4. It was reported that Bill Bland's QA presentation was

well received with an interest level half way between SRPO and BWIP;

5. Don Vieth stated that he is now the contracting officer for the NNWSI NTS contractors (Holms and Narver, Fennix and Scisson, REEC Co) and expects that he will soon add Sandia, LANL and LLNL to his list.

A brief licensing update was presented by Chris Pflum. The viewgraphs are enclosed.

There were three technical presentations. Bob Rundberg, LANL, presented the results, to date, of his work on fracture flow; C.F. Keller, LANL and Jerry Szymanski, DOE-WMPO spoke on the importance of coupled processes; and the LLNL group discussed the application of the EQ3/6 code to the high-level waste program. The viewgraphs are enclosed.

Bob Rundberg has shown, in the laboratory, that channeling is an important consideration in the movement of water through fractures. While this is not surprising intellectually, it is important that it has been shown experimentally. The bottom line of Rundberg's presentation was that fracture flow experiments, in-situ, will be difficult to design and will be expensive.

The presentation on coupled effects shows that the importance of the coupling of thermo-hydro-mechanical-chemical effects within the host rock is recognized by the NNWSI project. It is also recognized that the determination of the coupled effects is very difficult.

V. On Thursday, July 18, Mike Bell arrived in Las Vegas. I had dinner with Dr. Bell and he visited the Las Vegas Office. We discussed the project and the On-Site Representative Role in the Division.

VI. On Friday, July 19, Joe Bunting, Cathy Russell, and Paula Wade toured the Test Site. In the morning we visited "G" tunnel. This tour of the rock mechanics experiments in "G" tunnel was the most extensive tour I've participated in. We even had a demonstration of the "Alpine Miner".

After lunch we went through E-MAD. This very interesting facility is soon to be mothballed. The fuel rods that were used in the Climax experiment and the dry storage experiments are scheduled to be shipped to the Idaho facility.

Having completed the E-MAD tour we drove to drill hole wash, the site of the exploratory shaft, and to the top of Yucca Mountain.

VII. I'm enclosing some newspaper clippings about the shipment of radon contaminated soil from New Jersey to the Beatty low-level disposal facility. This is causing quite a flap in Las Vegas. It all started with the announcement that the soil would be held on a railroad siding in downtown Las Vegas while awaiting truck transport to Beatty. Legal action is planned and a temporary restraining order is expected to be issued until the legal aspects of the problem are sorted out. The City of Las Vegas, North Las Vegas, and Clark County are working together to bring suit against the railroad. The State's Attorney General has announced that the State of Nevada will not be a party to the action.

This is the first chance local governments have had to act against waste shipments through the County. I will keep you informed as the legal actions develop.



EA STATUS

STATUS OF COMMENT RESPONSE

- RESPONSE STATUS
- ISSUES RESOLVED SINCE LAST TPO MEETING
 - WASTE PACKAGE (GEOCHEMISTRY INTERACTION)
 - LINING FOR EX SHAFT MUCK PILE
 - POLICY ISSUES FOR LAND ACQUISITION & WATER RIGHTS
 - RESPONDED TO OCRWM REQUEST FOR MATERIALS FOR MARKEY'S HEARING
- UNRESOLVED ISSUES
 - GEOHYDROLOGY & TECTONICS RESPONSE
 - REPOSITORY DESCRIPTION
 - REPOSITORY EMPLOYMENT JUSTIFICATION
 - INCONSISTENCY IN WASTE RECEIPT RATES
 - CHAPTER 4 SOCIOECONOMIC GUIDANCE

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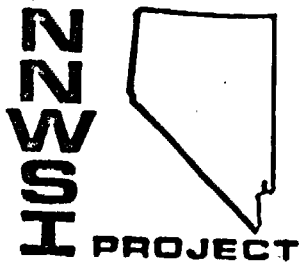


PROJECT

EA STATUS

STATUS OF COMMENT RESPONSE (CONT.)

- PERFORMANCE ASSESSMENT TIES FOR 33 GUIDELINES
(HQ LETTER REQUIRED REVISED GEOCHEMICAL CALCULATIONS)
- POLICY COMMENTS
 - * AIR FORCE
 - * WEAPONS TESTS
 - * OTHER



EA STATUS

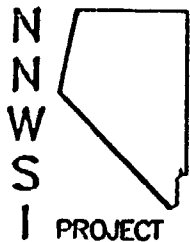
REMAINING SCHEDULE UNCERTAINTIES

- END OF COMMENT PERIOD (JULY 15 NNWSI PROJECT)
- ISSUE RESOLUTION MEETINGS
 - NOT SCHEDULED
 - STAFF CONFLICT FOR PREPARATION & ATTENDANCE
 - IF ADDITIONAL COMMENTS RESULT, A SCHEDULE SLIP IS EXPECTED



POST EA RELEASE

- STATE LEGAL CHALLENGE LIKELY FOR
 - GUIDELINES
 - GEOHYDROLOGY
 - TECTONICS
 - OFF SITE INSTALLATIONS & OPERATIONS
- RESPONSE TO CHALLENGE
 - DEPOSITIONS (WHO?)
 - WHITE PAPERS FOR ABOVE TOPICS



Los Alamos

FRACTURE FLOW

Bob Rundberg

RADIONUCLIDE TRANSPORT BY FLOW THROUGH FRACTURES

WHO CARES?

- NRC 10CFR60

"...Geochemical conditions that -(i) promote precipitation or sorption of radionuclides..."

" The performance confirmation program shall provide data which indicates, where practicable, whether--
Natural and engineered systems...are functioning as intended and anticipated. "

- EPA 40CFR191

"...the cumulative releases of waste to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall...." be less than limits.



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FRACTURE FLOW

10 CFR 960:

- *FAVORABLE CONDITION*

...Geochemical conditions that promote the precipitation, diffusion into the rock matrix, or sorption of radionuclides; inhibit the formation of particulates, colloids, inorganic complexes, or organic complexes that increase the mobility of radionuclides; or inhibit the transport of radionuclides by particulates, colloids, or complexes.



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FRACTURE FLOW

NRC COMMENTS TO THE EA:

- ...The assumption of porous flow is questionable because there is considerable uncertainty in the flux and flow mechanisms at Yucca Mountain...

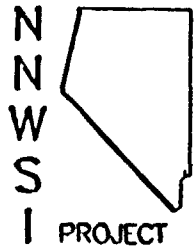


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FRACTURE FLOW

STATE OF NEVADA COMMENTS TO THE EA:

- ...The major question still remains as to how much diffusion will take place under conditions of fracture flow with velocities of several meters per day. Rainier Mesa tuffs are interpreted as having flow velocities of several meters per day with minimal changes in water chemistry from the soil zone to the tunnels...



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FRACTURE FLOW

STATE OF NEVADA COMMENTS TO THE EA:

- ...Fracture flow is ignored even though varying data support fracture flow in Yucca Mountain tuffs. The apparent lack of a multiple working hypothesis, which is basic to any scientific investigation, leads to ignoring many possibilities...



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FRACTURE FLOW

RADIONUCLIDE TRANSPORT BY FLOW THROUGH FRACTURES

WHO NEEDS IT?

- Performance Assessment

WHY DO THEY NEED IT?

- The fracture flow scenario reduces the effectiveness of adsorption.



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FRACTURE FLOW

THE CONSEQUENCES OF THE FRACTURE FLOW SCENARIO:

- A CONSERVATIVE APPROACH WOULD ONLY CONSIDER ADSORPTION ON THE FRACTURE SURFACES.
 - Considering only surface sorption leads to very small retardation factors.
- CONSIDERING MATRIX DIFFUSION ENHANCES ADSORPTION BY INCREASING THE SOLID PHASE VOLUME.
 - The effectiveness of matrix diffusion has not been quantitatively demonstrated.



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FRACTURE FLOW

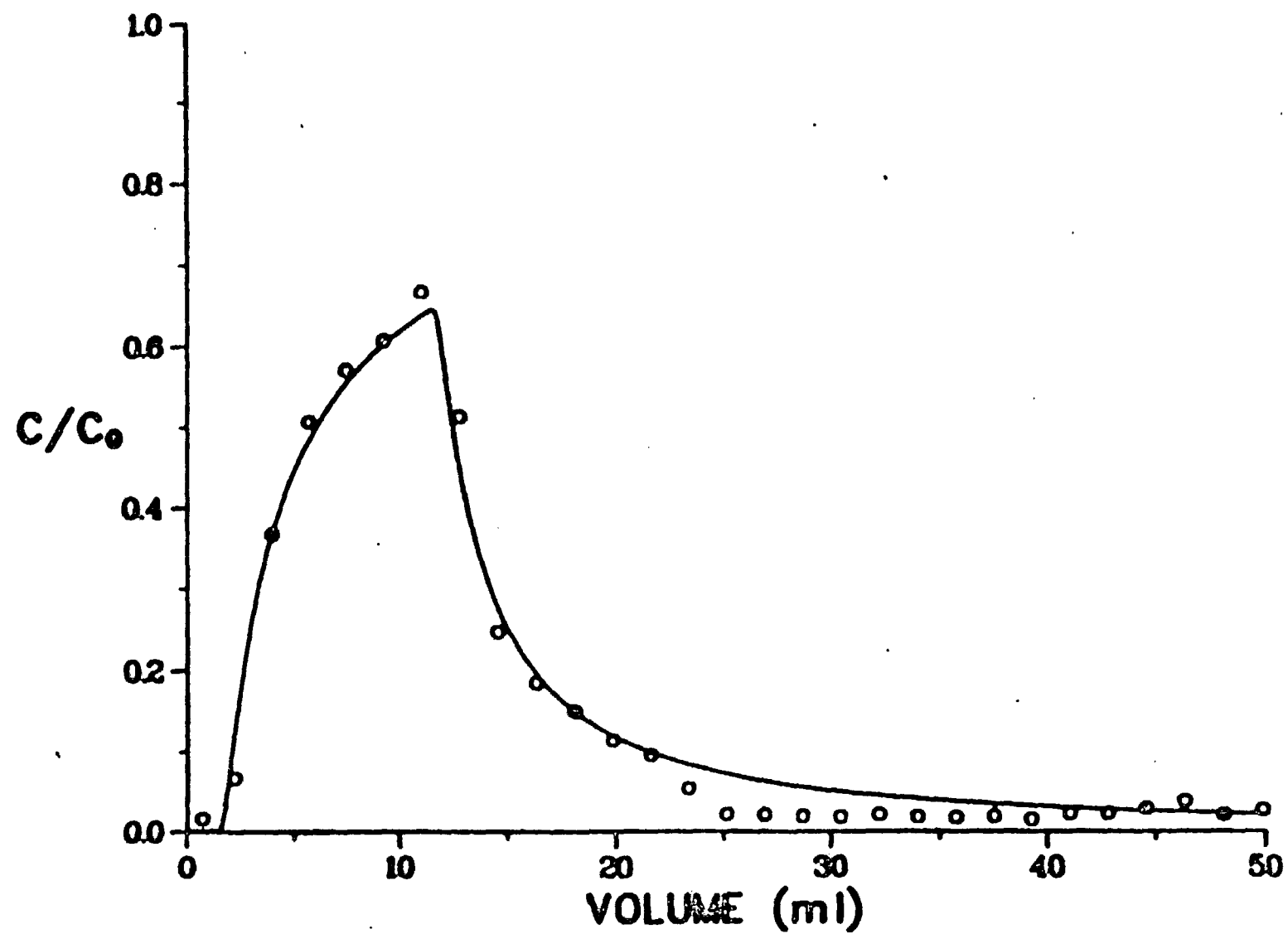
LABORATORY EXPERIMENTS DO NOT SUPPORT THE SIMPLEST VIEW
OF MATRIX DIFFUSION:

- The breakthrough of radionuclides occurs with an effective K_d many orders of magnitude smaller than established by batch sorption techniques based on the matrix diffusion model.

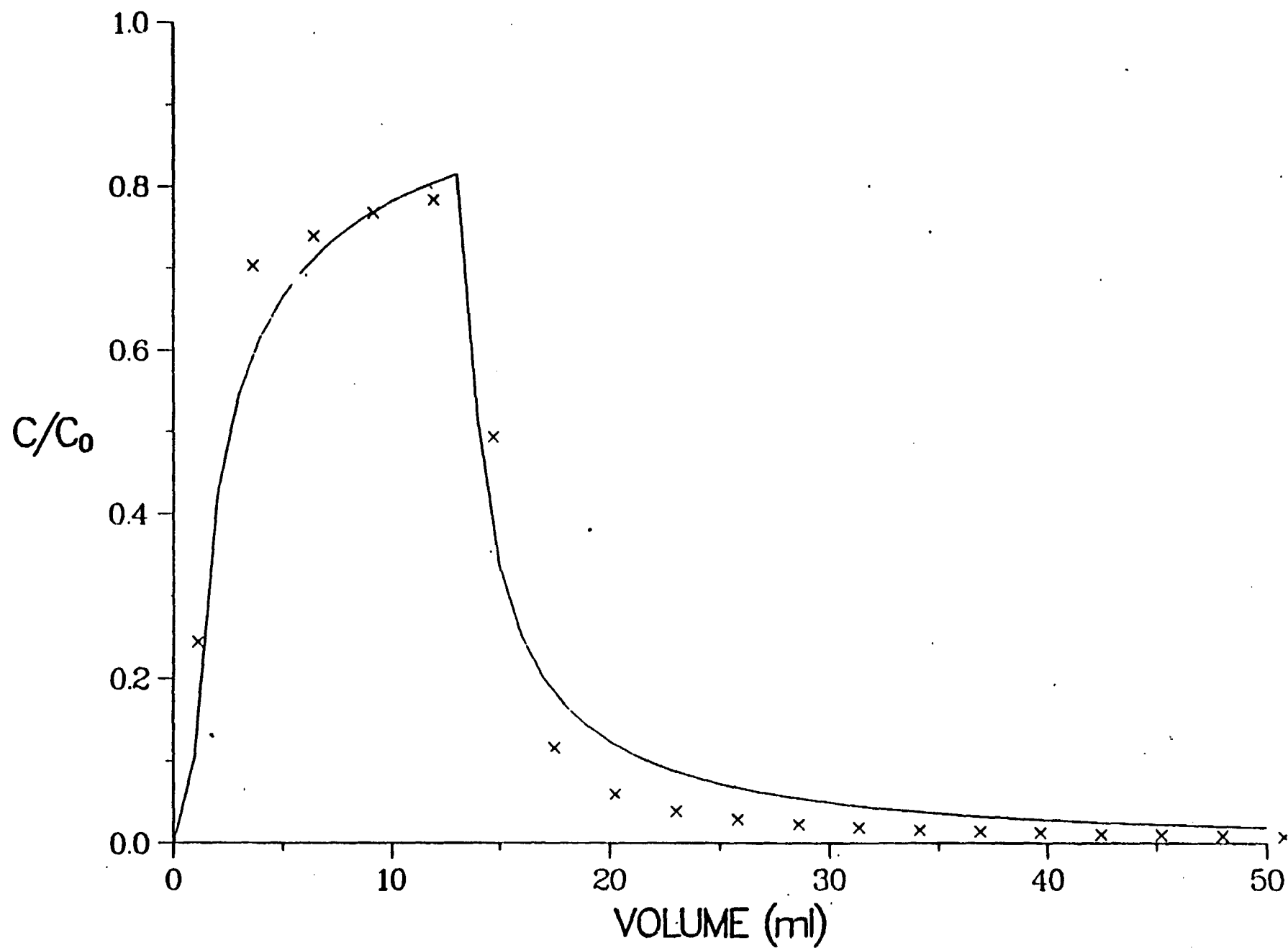
Ref. Erickson and Neretnieks, Rundberg et al.

- The explanation for this disagreement has yet to be explained!

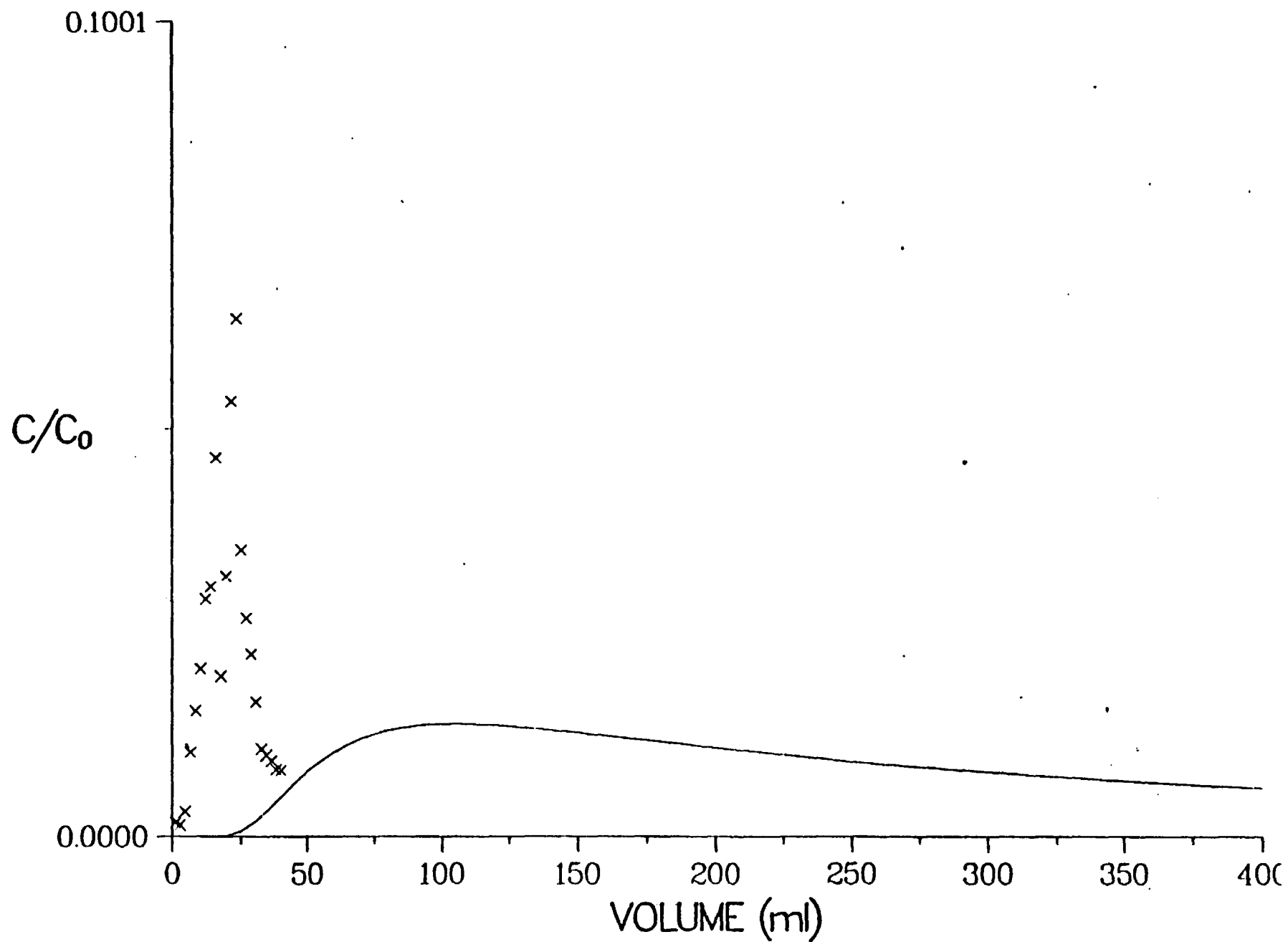
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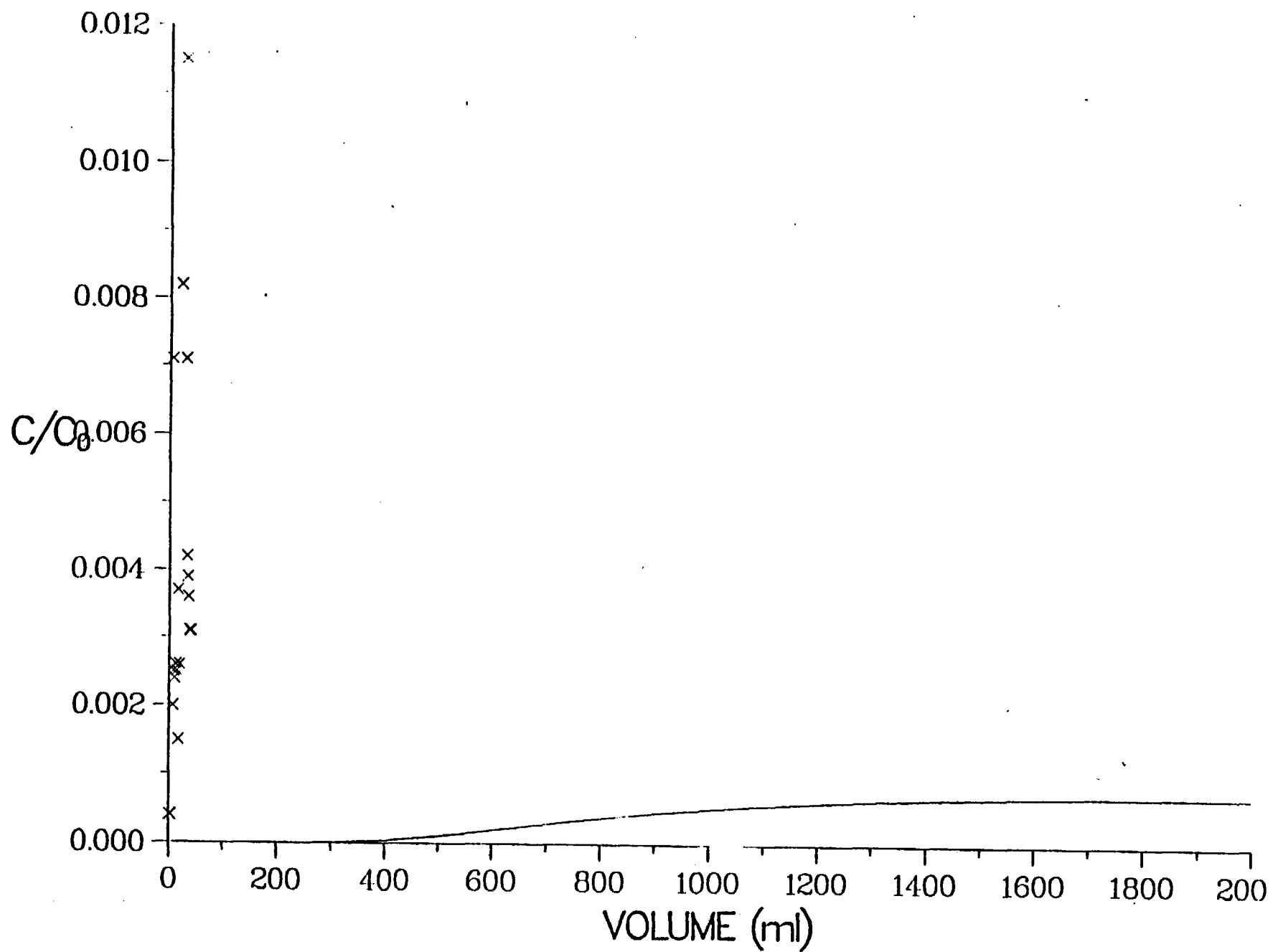
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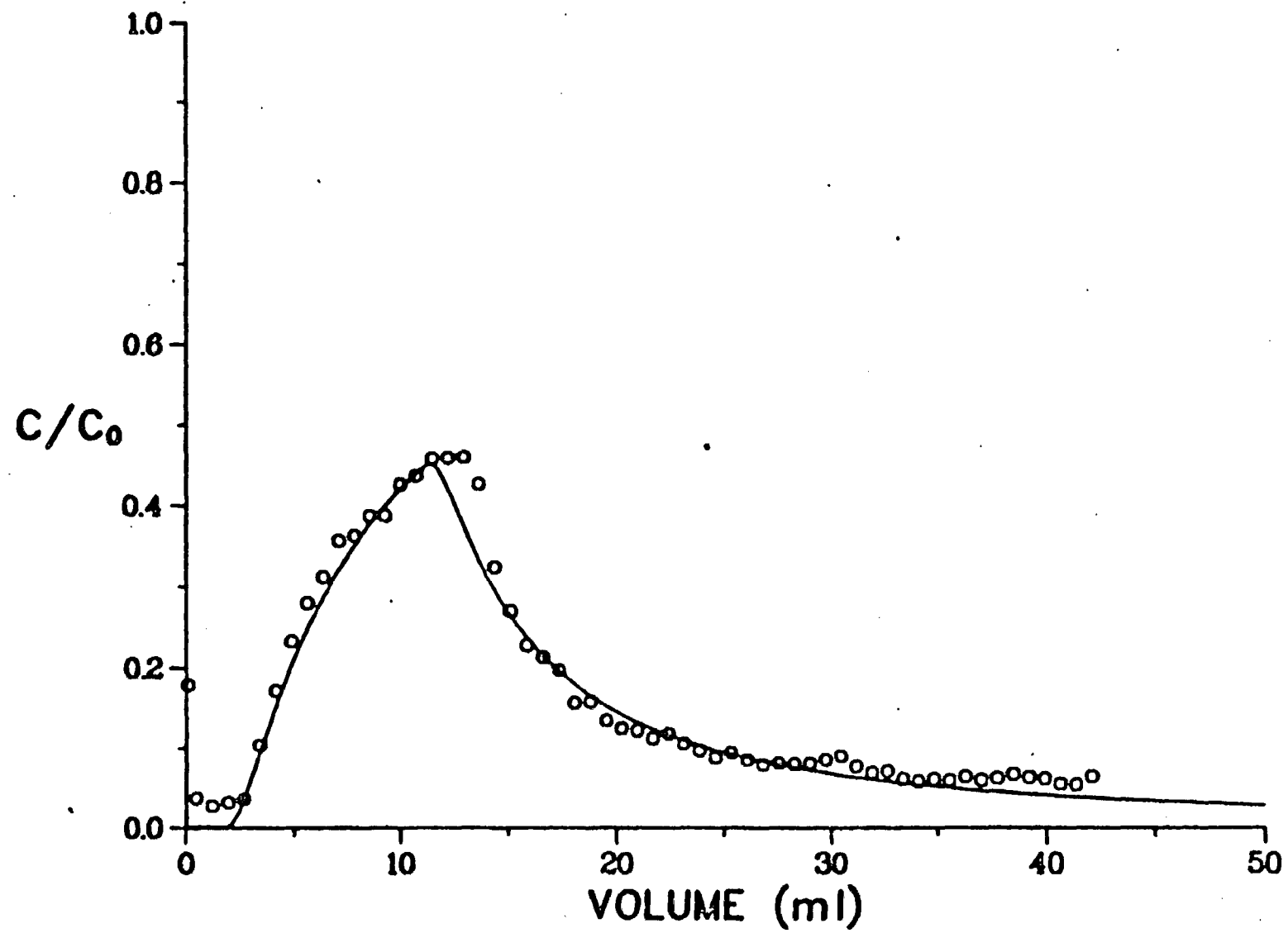
STRONTIUM ELUTION GU3-2114



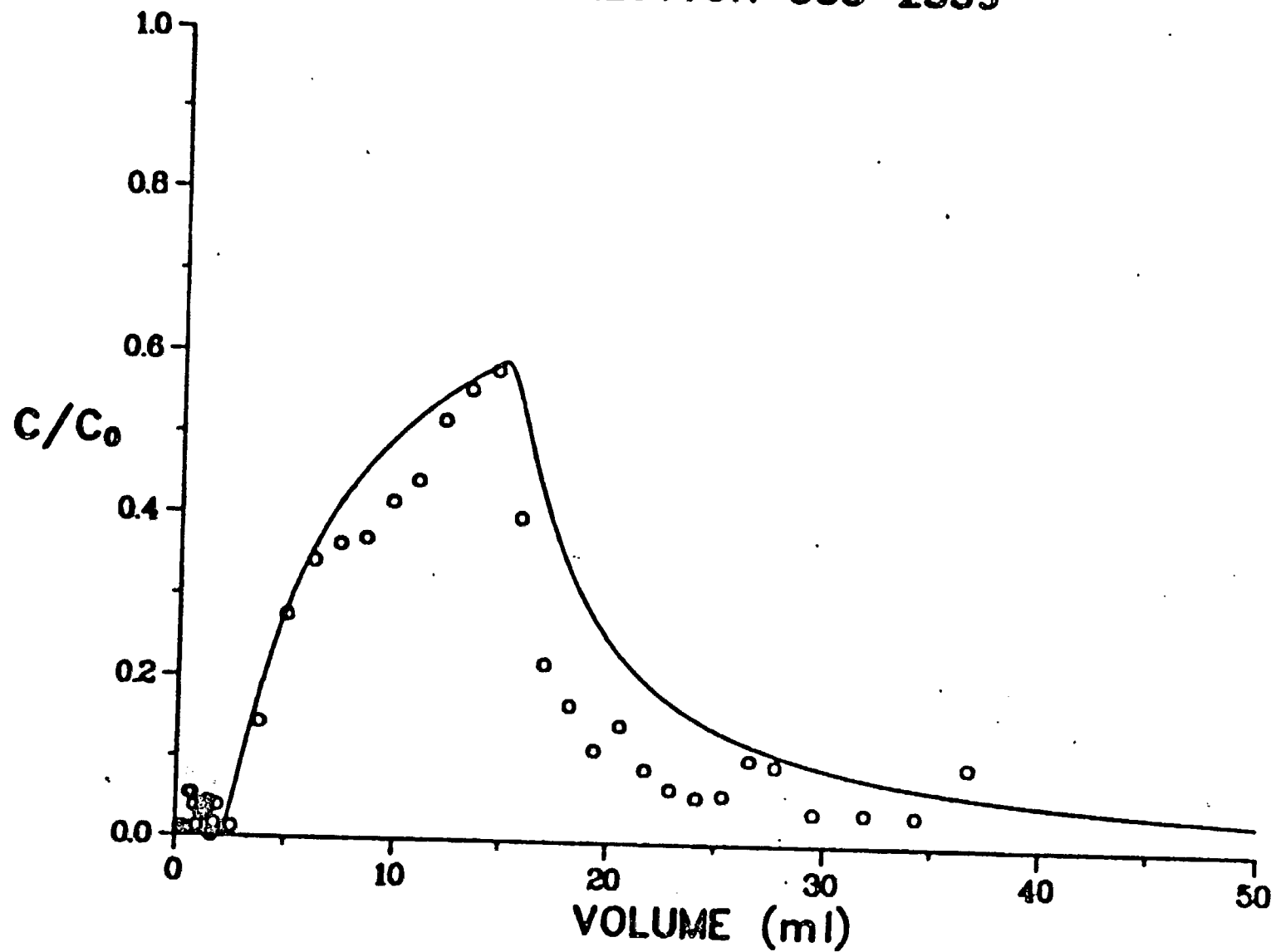
BARIUM ELUTION GU3-2114



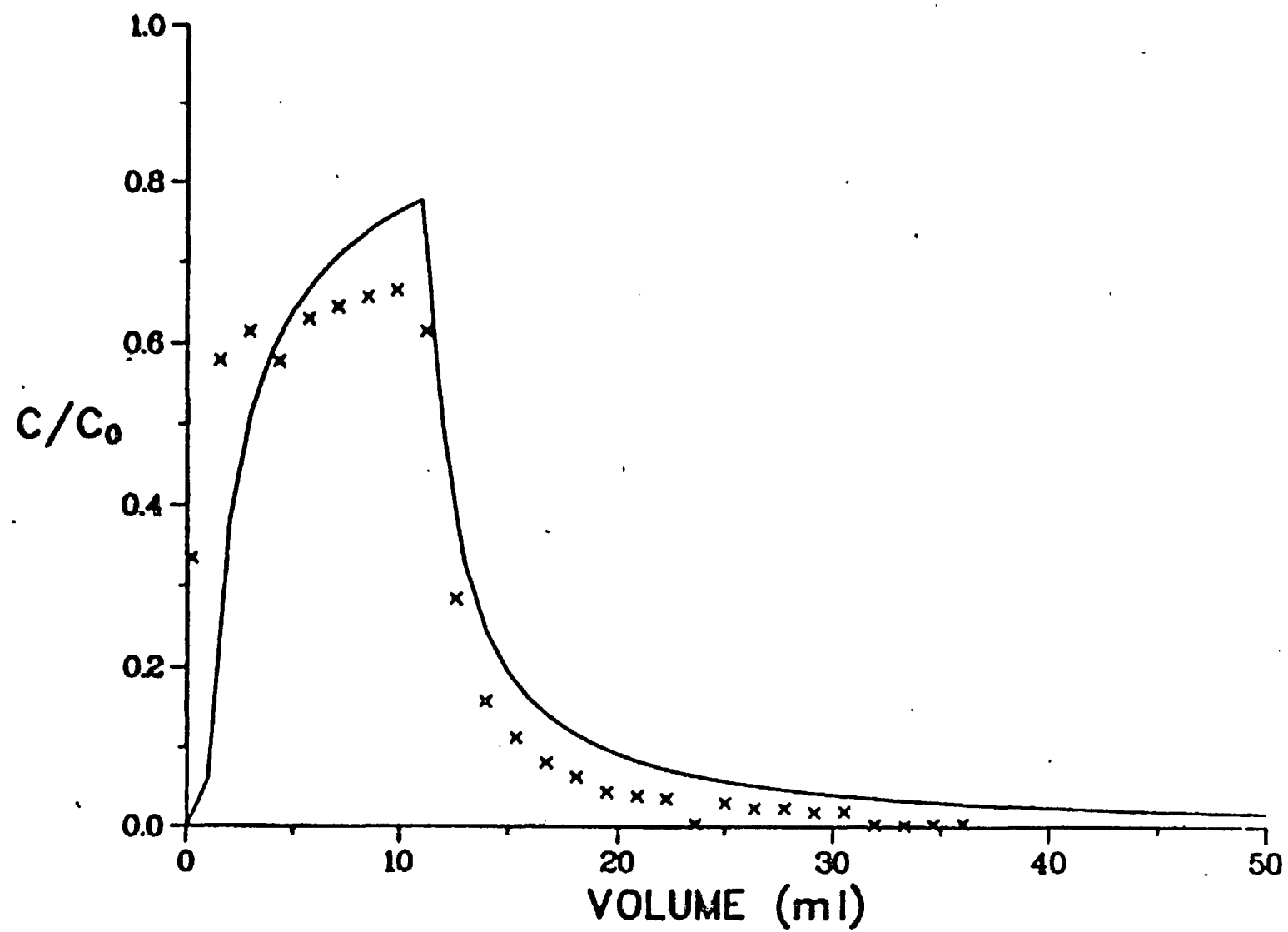
HTO ELUTION GU3-2359



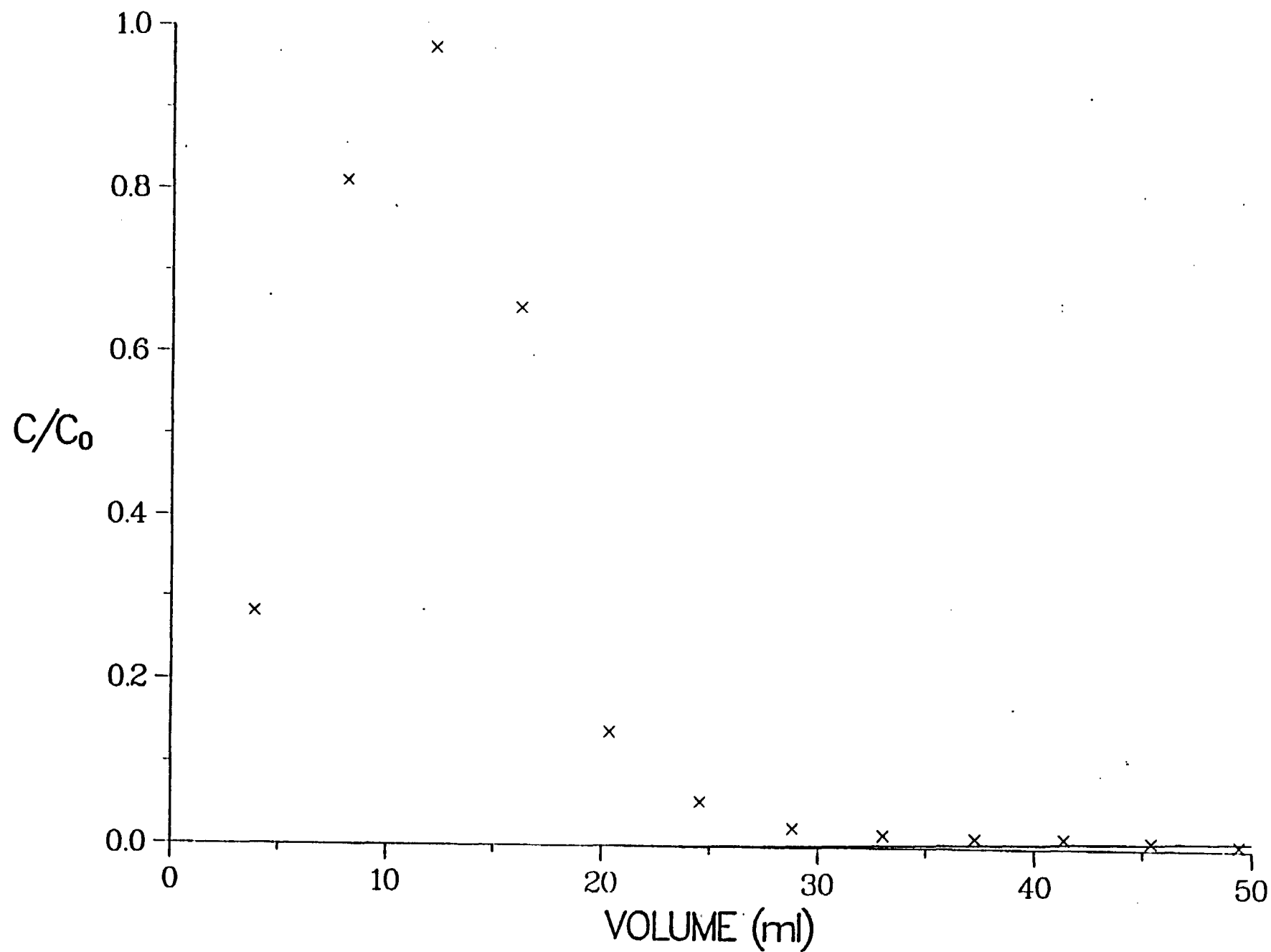
HTO ELUTION GU3-2359

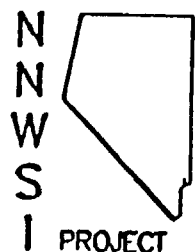


PERTECHNETATE ELUTION GU3-2359



STRONTIUM ELUTION GU3-2359



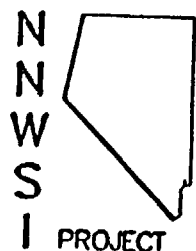


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FRACTURE FLOW

PROBABLE CAUSES FOR THE OBSERVED DISAGREEMENT BETWEEN LABORATORY EXPERIMENTS AND THE MATRIX DIFFUSION MODEL:

1. Severe channeling, thus greatly reducing the effective surface area of the fracture.
2. The uneven distribution of adsorbing minerals; i.e., the fracture surfaces are depleted in clays.
3. Adsorption kinetics (This cause is less plausible because data from other experiments support diffusion-limited adsorption.)
4. Surface diffusion (This mechanism, although proposed by Neretnieks and Rasmussen, is dubious because it is exotic and based on an effect observed only in the adsorption of gases on metal surfaces.)



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FRACTURE FLOW

PRESENT EVALUATION OF POSSIBLE CAUSES FOR THE LACK OF AGREEMENT BETWEEN THEORY AND EXPERIMENT

- ADSORPTION KINETICS

Not likely for the following reasons:

1. Fluid velocities in recent experiments have been slowed to 8×10^{-4} cm/sec.
2. Adsorption kinetics have been shown to be consistent with diffusion-limited rates.
3. Mass transfer broadening is not evident.



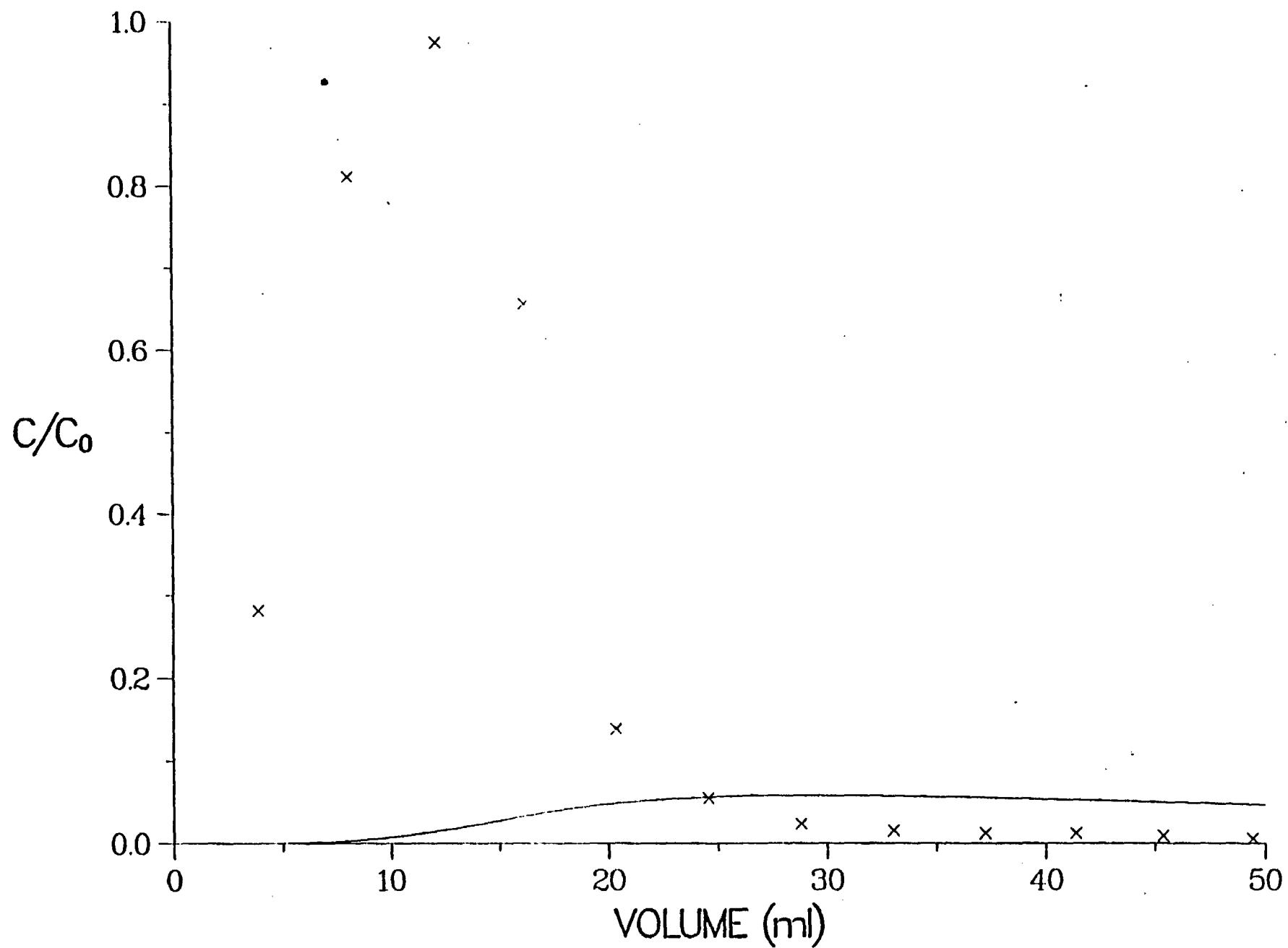
Los Alamos

FRACTURE FLOW

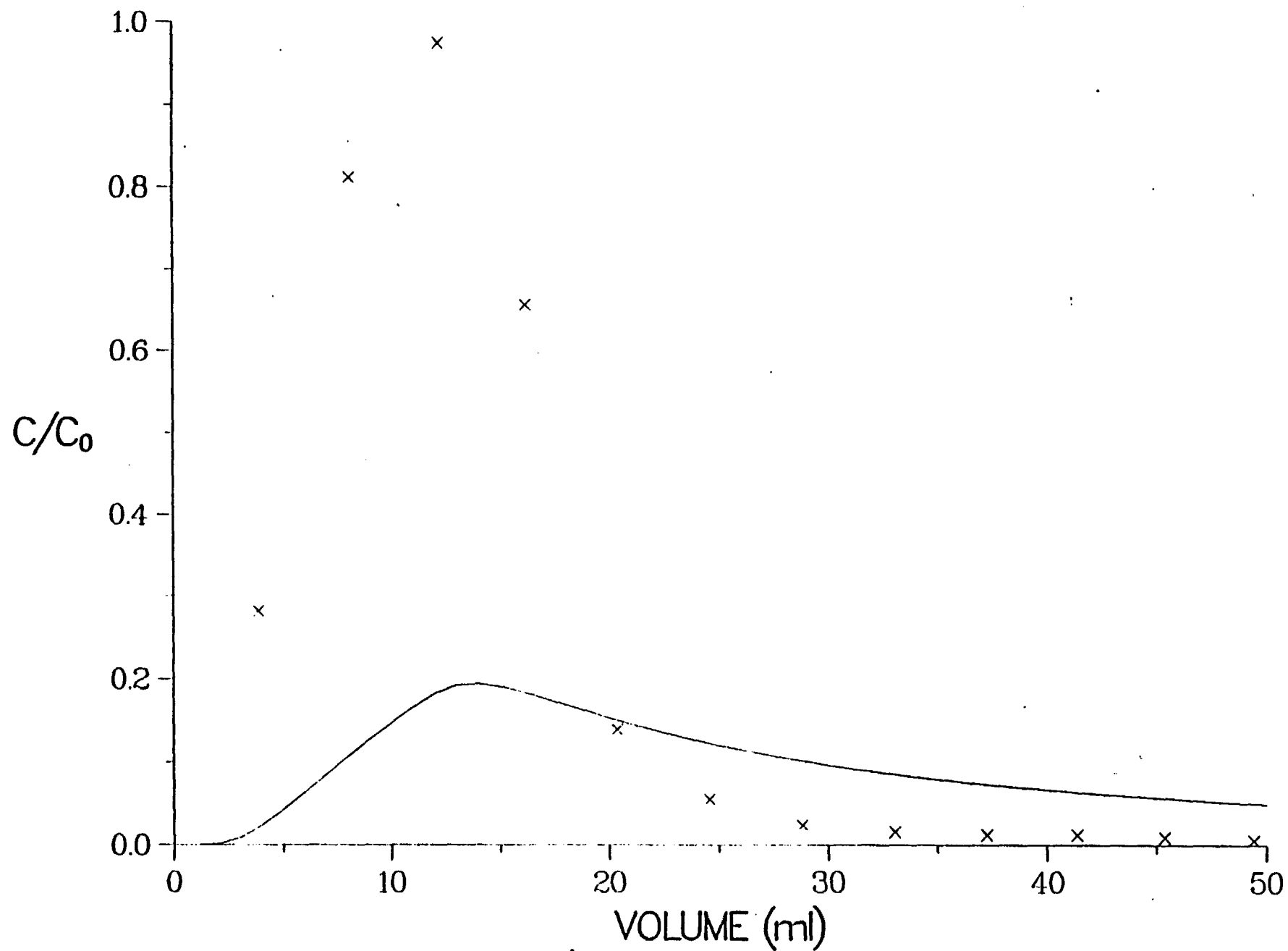
PRESENT EVALUATION OF POSSIBLE CAUSES FOR THE LACK OF AGREEMENT BETWEEN THEORY AND EXPERIMENT

- CHANNELING
 - Has been observed through autoradiography.
 - The sensitivity of retardation to channeling has been demonstrated using TRACR3D.
 - A stochastic model applicable to channeling is being developed.

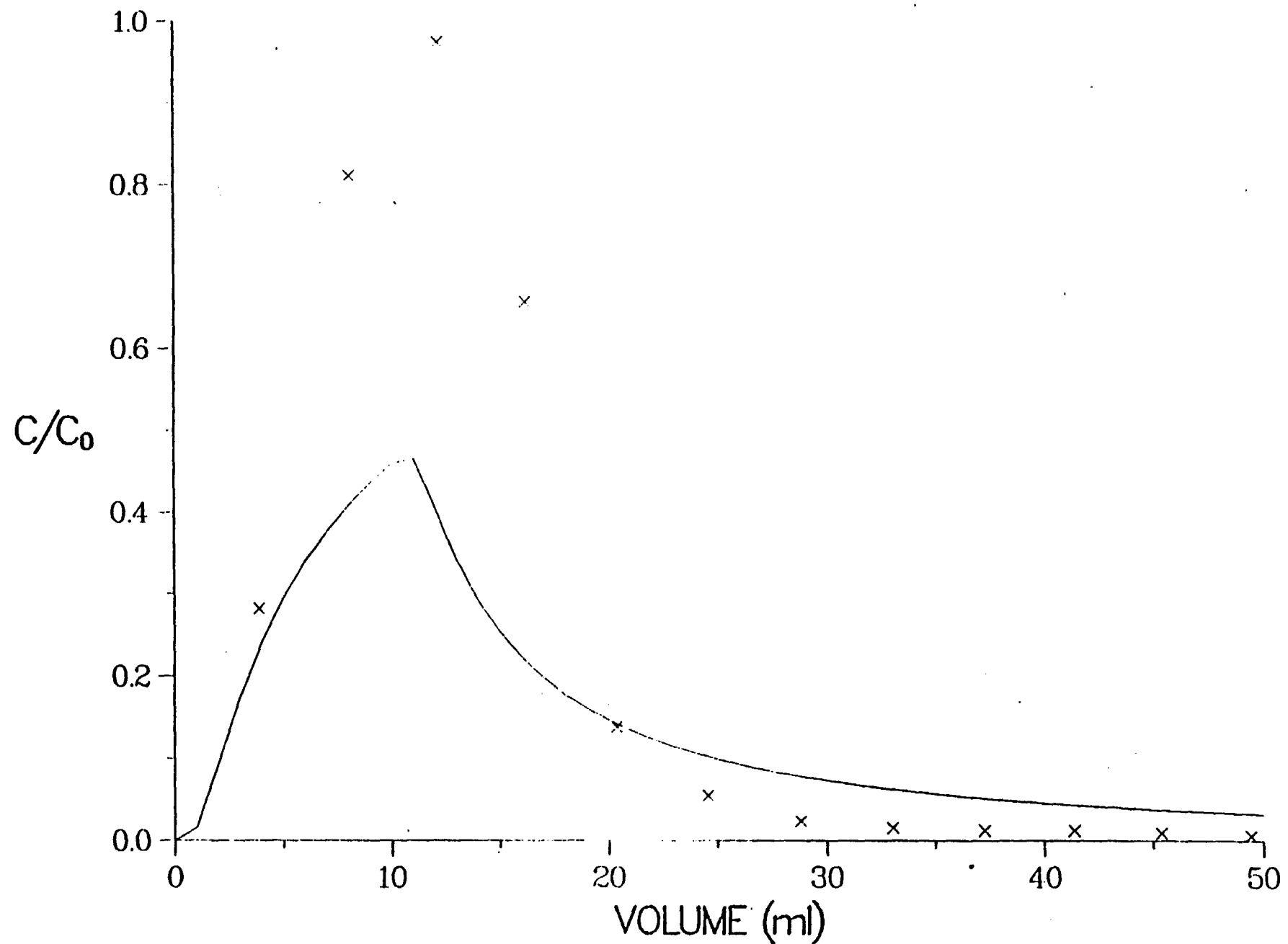
STRONTIUM ELUTION GU3-2359-W=1/2



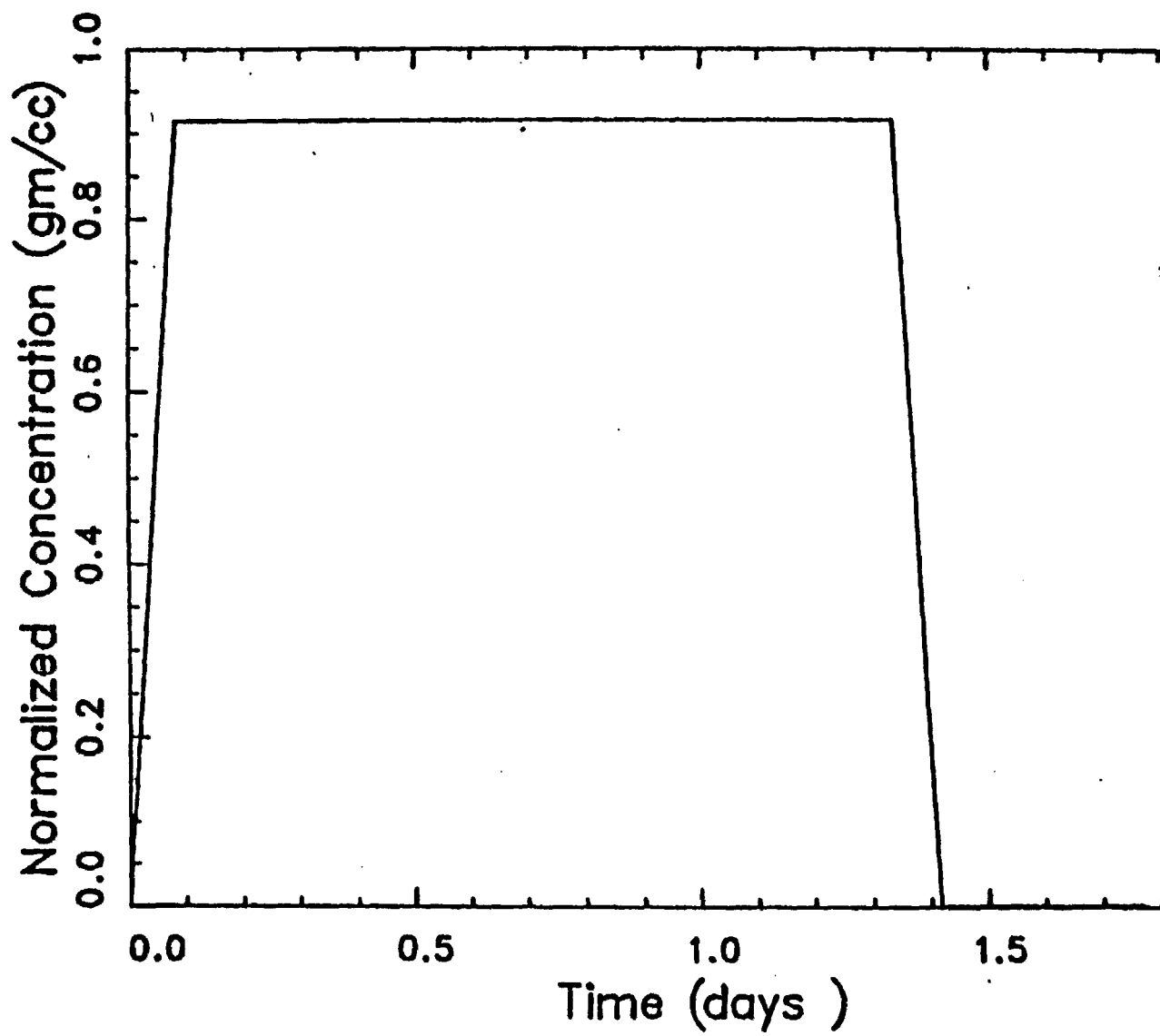
STRONTIUM ELUTION GU3-2359-W=1/4



STRONTIUM ELUTION GU3-2359-W=1/8



bob's fracture experiment 1.38 mm channel





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FRACTURE FLOW

PRESENT EVALUATION OF POSSIBLE CAUSES FOR THE LACK OF AGREEMENT BETWEEN THEORY AND EXPERIMENT

- UNEVEN DISTRIBUTION OF SORBING MINERALS
 - A depletion of clays or other sorbing minerals from the fracture surface could lower the retardation.
 - There is no evidence at present to support this hypothesis.
 - A stochastic model for the distribution of minerals could be developed if necessary.



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FRACTURE FLOW

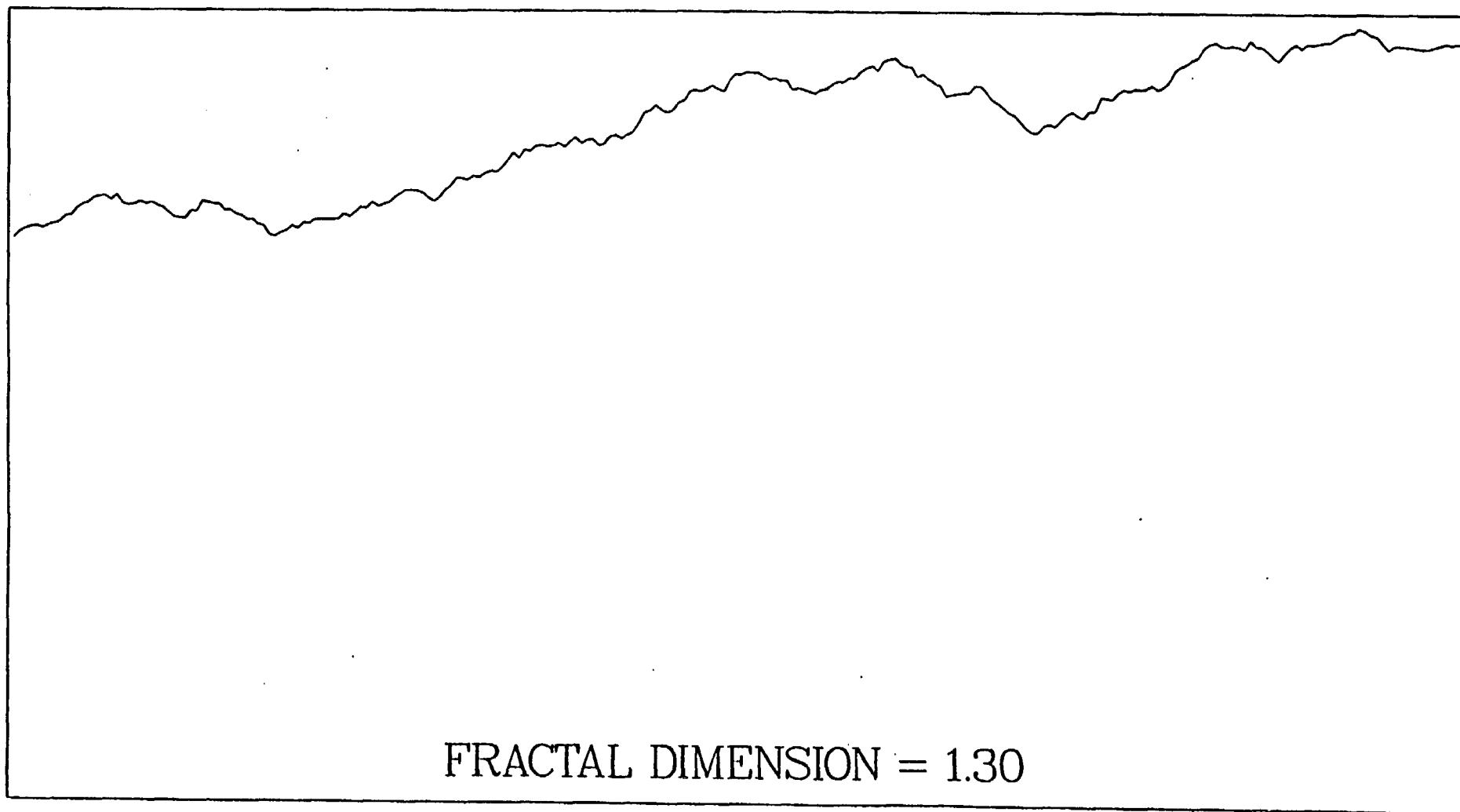
MODELING APPROACH REQUIRED TO DESCRIBE CHANNELING AND OTHER HETEROGENEOUSLY DISTRIBUTED PROPERTIES:

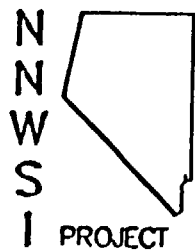
- Stochastic functions are desirable.
- It should be determined if the properties of tuff are self-similar.
- If the heterogeneous properties of tuff are self--similar, then the channeling on large scales can be predicted. In addition, if the properties are self-similar, effects such as channeling will be more severe at a larger scale.



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FRACTURE FLOW





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FRACTURE FLOW

THE CONSEQUENCES OF CHANNELING TO FIELD TESTS OF RADIONUCLIDE TRANSPORT

1. IF CHANNELING HAS SELF-SIMILAR PROPERTIES IT WILL BECOME MORE SEVERE AT LARGER SCALES.
 - a. Many geologic properties are self-similar.
 - b. Channeling has hindered the Stripa transport experiments.
2. CHANNELING WILL HINDER FRACTURE FLOW EXPERIMENTS:
 - a. Only a small fraction of the injected fluid, if any, is likely to be intercepted by a single sampling point.
 - b. Even if the fluid is sampled successfully, the flow path is unknown, making the interpretation of any results difficult or impossible by conventional analysis.

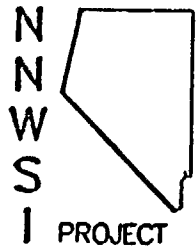


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FRACTURE FLOW

THE CONSEQUENCES OF CHANNELING TO FIELD TESTS OF RADIONUCLIDE TRANSPORT

3. AN EXPERIMENT DESIGNED TO BE SUCCESSFUL WILL BE EXPENSIVE.
4. IF CHANNELING REDUCES THE EFFECTIVE RETARDATION OF RADIO-NUCLIDES, THEN SUFFICIENTLY LARGE TRANSPORT EXPERIMENTS MUST BE CONSIDERED.



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FRACTURE FLOW

FIELD DATA REQUIRED TO MODEL

CHANNELING OR OTHER NONLINEAR EFFECTS:

1. The surface topography of fractures
2. The displacement of faults and fractures
3. The distribution of adsorbing minerals
4. The distribution of secondary minerals deposited by fracture fluids



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FRACTURE FLOW

DERIVED DATA REQUIRED FOR MODELING:

1. The Hausdorf-Besicovitch dimension of fracture surfaces and distributions.
2. Scale limits for the fractional dimensions.
3. The dimension of flow paths which result from the flow of fluids between fractional brownian surfaces.



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FRACTURE FLOW

THE CONSEQUENCES OF CHANNELING AND HETEROGENEOUSLY DISTRIBUTED PROPERTIES ON PERFORMANCE ASSESSMENT

1. Translational symmetry may not be a valid assumption, i.e., the REV concept is dead.
2. The porous flow approximation will be invalid unless an REV can be demonstrated.
3. If dilational invariance is valid, then large scales can be modeled. Depending on the fractional dimension, however, uncertainties will become very large when data are extrapolated to very large scales.
4. Stochastic models are necessary to bound radionuclide transport.

TPO
PRESENTATION
07/25/85

SCP PRESENTATION

STATUS OF DATA AND DESIGN CHAPTERS	M. TEUBNER
POINTS OF INTEREST FROM IRC MEETINGS	J. YOUNKER
CHAPTER 8 STATUS	D. JORGENSEN
SECTION 8.3 REVIEW PROCESS	D. JORGENSEN
SCP SCHEDULE	M. TEUBNER
ISSUES HIERARCHY UPDATE	J. YOUNKER

STATUS OF DATA AND DESIGN CHAPTERS

<u>CHAPTER</u>	<u>COMMENTS</u>
1	TEXT RECEIVED, BEING REVIEWED BY TDWGC
2	COMMENTS BEING RESOLVED BY SNL, DUE BACK BY 8/2
3	IN INTERNAL REVIEW. MEETING 7/29-31
4	DUE TO BE RECEIVED 7/26
5	IN INTERNAL REVIEW. MEETING 8/1-2
6	TEXT RECEIVED, BEING REVIEWED BY TDWGC
7	IRC MEETING HELD 7/17-19. COMMENTS TO BE DELIVERED TO LLNL 7/29

**TECHNICAL DATA AND DESIGN CHAPTERS
CONCERNS FROM INITIAL REVIEWS**

- **COMPLIANCE WITH THE ANNOTATED OUTLINE**
- **COMPLIANCE WITH THE STYLE GUIDE**
- **CROSS-REFERENCING: WITHIN CHAPTER
BETWEEN TD&D CHAPTERS
WITH CHAPTER 8 (8.3)**
- **MORE EXTENSIVE REFERENCING**
- **REFERENCES, GLOSSARY, ABBREVIATIONS**
- **COPYRIGHT CLEARANCES**

7-25-85
TPO MEETING

IRC STATUS

- 0 CHAPTERS 2 & 7 THROUGH IRC REVIEW
- 0 AUTHOR ROLE HAS CHANGED -- AUTHOR OR REPRESENTATIVE REQUESTED AT MEETING TO ANSWER QUESTIONS & HEAR COMMENTS

CHAPTER 2

- 0 OVERRIDING COMMENT WAS "EXPLAIN WHY WE CARE FROM THE STANDPOINT OF PERFORMANCE"
- 0 IDENTIFY UNCERTAINTY IN DATA AND INTERPRETATIONS
- 0 REVIEWS ARE DIFFICULT WITHOUT REFERENCES
- 0 REVIEWS ARE DIFFICULT DUE TO CROSS-REFS & LARGE TRACKING JOB IS DEFINED IN MARK-UP
- 0 NEED TO EXPLAIN "HISTORICAL PERSPECTIVE" OF DATABASE
- 0 NEED TO REFERENCE OTHER PROJECT WORK
- 0 SEVERAL SECTIONS TO BE RE-REVIEWED

CHAPTER 7

- 0 NEED BETTER TIE TO ISSUES HIERARCHY
- 0 VERY DIFFERENT FROM CHAPT. 6 --
NOT A DESIGN CHAPTER
- 0 NEED GR/MGDS IN DESIGN BASIS
- 0 COPPER CANISTER
- 0 PROGRAM CONSISTENCY

CHAPTER 8 STATUS

8.1 RATIONALE

DRAFT DUE 8/9

8.2 ISSUES AND INFORMATION NEEDS

DRAFT DUE 8/9

8.3 PLANNED TESTS, ANALYSES, AND STUDIES

DRAFT DUE 10/4

INDO'S 60% COMPLETED

PROJECTED COMPLETION DATES FOR SUBSECTIONS:

8.3.1 9/23

8.3.2 8/06

8.3.3 8/06

8.3.4 9/30

8.3.5 9/06

8.4 PLANNED SITE PREPARATION ACTIVITIES

DRAFT SUBMITTED 7/12

REVIEWED AND RETURNED TO AUTHOR FOR REPAIRS

8.5 MILESTONES, DECISION POINTS, SCHEDULE

DRAFT DUE 10/4

8.6 QUALITY ASSURANCE PROGRAM

DRAFT SUBMITTED 5/8

REQUIRES ADDITIONAL TECHNICAL AND QA PROCEDURES FOR COMPLETION

8.7 DECONTAMINATION AND DECOMMISSIONING

DRAFT SUBMITTED 5/20

QUESTION #1

**SHOULD THE TPO'S SERVE AS THE INTERNAL REVIEW
COMMITTEE FOR SECTIONS 8.1 AND 8.2?**

- o 8.1 AND 8.2 ARE A STATEMENT OF NNWSI
PROJECT PHILOSOPHY**
- o 8.1 AND 8.2 PRESENT THE RATIONALE AND LOGIC
FOR WHAT THE NNWSI PROJECT PLANS TO DO
DURING SITE CHARACTERIZATION PHASE**

SECTION 8.3 REVIEW PROCESS

- o AS PRACTICAL, PARTS OF 8.3 WILL BE INTERNALLY REVIEWED WITH THEIR CORRESPONDING DATA/DESIGN CHAPTERS
 - 8.3.1 HYDROLOGY WITH CHAPTER 3 7/29
 - 8.3.1 CLIMATOLOGY WITH CHAPTER 5 8/1
 - 8.3.1 GEOLOGY WITH CHAPTER 1 9/9
 - 8.3.1 GEOCHEMISTRY WITH CHAPTER 4 9/11
 - 8.3.2 AND 8.3.3 WITH CHAPTER 6 8/21
- o 8.3.1 AND 8.3.5 WILL UNDERGO SEPARATE INTERNAL REVIEWS ON 10/3 AND 9/16, RESPECTIVELY
- o SECTION 8.3 IN ITS ENTIRETY WILL UNDERGO INTERNAL REVIEW (11/4) AND HQ REVIEW (12/11)
- o IS IT DESIRABLE AND PRACTICAL TO STAGE A WORKSHOP (WRITE-IN) FOR 8.3?

QUESTION #3

HOW AND WHEN WILL THE PROJECT DEVELOP A SURFACE-BASED TEST PLAN?

- o HQ IS PREPARING ANNOTATED OUTLINES FOR AN ESTP, PAP, AND SBTP
- o A SBTP WILL PROVIDE A BALANCE IN THE TREATMENT OF ES TESTS AND NON-ES TESTS
- o THE CONTENT OF 8.3 DEPENDS ON THE EXISTENCE OF A SBTP
- o SHOULD WE HAVE A SBTP COMMITTEE SIMILAR TO THE ESTP COMMITTEE?
- o ACTION ITEM:

SCP SCHEDULE

- o NEW SCHEDULE DEVELOPED 7/22/85
- o MINOR CHANGES BASED ON POTENTIAL CONFLICTS
BETWEEN EA, SCP, NRC MEETINGS
- o COMMENTS:
 - INITIAL INPUT DATES SAME
 - IRC MEETINGS BASICALLY SAME
 - HQ REVIEW MEETINGS SLIGHTLY DIFFERENT
(MORE CONSOLIDATED)
 - HQ CONCURRENCE DATE STILL 3/28/86
- o NEW SCHEDULE

July 22, 1985
10:45 a.m.

SCP SCHEDULE

Chapter/ Section	Draft Input	Internal Distr.	Review Mtg.	CRAP 1	HQ Review Distr.	Mtg.	CRAP 2
2		-	-	7/2 - 8/16	8/19	8/29-30	9/2 - 10/25
7	6/21	6/24	7/17-19	7/22 - 9/20	9/23	10/8-9	10/14 - 11/22
3	6/16	7/19	7/29-31	8/5 - 9/20	9/23	10/10-11	10/14 - 11/22
8.3.1 Hyd	7/22	7/24	7/29-31	8/5 to USGS	-	-	- -
5	7/17	7/19	8/1-2	8/5 - 9/20	9/23	10/9	10/14 - 11/22
8.4,8.7	6/28	8/12	8/19-20	8/26 - 9/27	9/30	10/9	10/14 - 11/22
6	7/19	8/12	8/21-23	8/26 - 9/27	9/30	10/10-11	10/14 - 12/6
8.3.2	8/6	8/12	8/21-23	8/26 to SNL	-	-	- -
8.3.3	8/6	8/12	8/21-23	8/26 to SNL	-	-	- -
8.6	8/6	8/12	8/22-23	8/26 - 9/20	9/23	10/8	10/14 - 12/6
0	8/8	8/23	9/3-4	9/9 - 10/11	10/14	10/28	10/30 - 12/6
8.1,8.2	8/9	8/23	9/3-5	9/9 - 10/11	10/14	10/28	10/30 - 12/6
1	7/19	8/26	9/9-11	9/16 - 10/18	10/21	10/29-30	11/4 - 12/6
8.3.1 Geo	8/2	8/26	9/9-11	9/16 to USGS	-	-	- -
4	7/26	8/26	9/11-13	9/16 - 10/18	10/21	10/31-1	11/4 - 12/6
8.3.1 Chem	8/2	8/26	9/11-13	9/16 to LANL	-	-	- -
8.3.5	8/16	9/2	9/16-17	9/19 to SNL	-	-	- -
8.3.1	9/23	9/26	10/3-4	10/7 to SAIC	-	-	- -
8.3, 8.5	9/23	10/21	11/4-8	11/11 - 11/29	12/2	12/11-13	12/16 - 1/10

Total Document Consolidation	1/13 - 1/17 (SAIC)
HQ/Internal Reviews	1/20 - 2/7 (HQ/NNWSI Project)
Comment Clarification & Consolidation	2/10 - 2/14 (HQ)
Comment Resolution	2/17 - 2/28 (SAIC)
Production	3/3 - 3/14 (SAIC)
HQ Approval	3/17 - 3/28 (HQ)

CRAP = Comment Response & Distribution

UPDATE ON ISSUES HIERARCHY

- 0 SUGGESTED CHANGES WERE RECEIVED AND LINE-IN/LINE-OUT VERSION DISTRIBUTED ON JULY 10

(SPLIT POTENTIAL EFFECTS IN'S FROM 1 TO 3; ADDED DESIGN CONCEPTS TO PERFORMANCE IN'S; MOVED BACKGROUND RADIATION FROM ISSUE 2.6 TO 2.7)

- 0 COMMENTS WERE REQUESTED ON CHANGES

LANL: OBJECTED TO PHRASE "DESIGN CONCEPTS" AND SUGGESTED "DESIGN INFORMATION" OR "REFERENCE DESIGN"

ALSO INDICATED THAT 1.15 DOES NOT NEED DESIGN INFORMATION

NO OTHER COMMENTS TO DATE

- 0 KEY ISSUE III IS STILL UNDER REVISION. -- SOME INFORMATION NEEDS REMAIN TO BE WRITTEN AND THE ENTIRE SET WILL NEED CONDENSATION & REVIEW

FUTURE PLANS FOR ISSUES HIERARCHY

- O REQUEST THAT COMMENTS/SUGGESTIONS BE SENT TO J. YOUNKER
- O SAIC WILL COMPLETE KEY ISSUE III IN'S AND GET THEM OUT FOR REVIEW
- O 8.2 -- WILL BE WRITTEN TO "CURRENT VERSION" OF ISSUES HIERARCHY
- O ATTACHED LETTER WAS SENT TO R. STEIN ON 7-12-85 SUGGESTING NNWSI TAKE LEAD IN PLANNING FOR GENERIC WORKSHOP WITH NRC IN OCT-NOV TIMEFRAME



Department of Energy

Nevada Operations Office

P. O. Box 14100

Las Vegas, NV 89114-4100

JUL 12 1985

Ralph Stein, Acting Director, Engineering & Licensing Division; Office of
Geologic Repositories, DOE/HQ (RW-23), FORSTL

SITE CHARACTERIZATION PLAN (SCP) ISSUE RESOLUTION STRATEGY AND DATA NEEDS

The Nevada Nuclear Waste Storage Investigation (NNWSI) Project strongly supports the idea of holding a workshop with the Nuclear Regulatory Commission (NRC) on generic approaches to issue resolution strategies. Such a meeting was tentatively established for the October-November timeframe at the May 30, 1985 Department of Energy (DOE)/NRC Management Meeting. We encourage your office to move forward with plans for that meeting.

One major objective of such a meeting could be to gain the NRC's concurrence with an issues hierarchy approach to the identification and resolution of licensing questions. This could be of substantial benefit to the program as it would provide a basis for agreement between the NRC and the DOE on data and information needed to meet licensing requirements. The philosophy that has been developed in the NNWSI Project Issues Hierarchy is that each tier in the hierarchy (data-analyses-parameters, information needs, issues, key issues) displays all of the relevant material that is required to resolve the questions of the next higher tier in the hierarchy. This leads to an Issues Hierarchy that can serve as a checklist against which progress toward resolution of licensing issues can be evaluated.

Because we consider this topic to be extremely important, we are prepared to commit the necessary NNWSI Project resources to develop and participate in the workshop. We will prepare and submit a preliminary draft workshop agenda to you for your consideration before July 31.

A handwritten signature in dark ink, reading "Donald L. Vieth".

Donald L. Vieth, Director
Waste Management Project Office

WMPO:JSS-1260

cc:

M. D. Voegele, SAIC, Las Vegas, NV
M. E. Spaeth, SAIC, Las Vegas, NV
M. A. Glora, SAIC, Las Vegas, NV
J. L. Younker, SAIC, Las Vegas, NV
M. B. Blanchard, WMPO, DOE/NV
C. L. Hanlon, DOE/HQ (RW-24), FORSTL
W. J. Purcell, DOE/HQ (RW-20), FORSTL
V. J. Cassella, DOE/HQ (RW-22), FORSTL



LICENSING UPDATE

JULY 24, 1985

NNWSI



PROJECT

- **NRC MEETINGS WITH;**
 - **NNWSI PROJECT**
 - **DOE/HQ**
- **DRAFT 6 OF EPA STANDARD (40CFR191)**
- **SECRETARY OF ENERGY'S PRELIMINARY DETERMINATION OF SITE SUITABILITY**

**NSN
HSH**



PROJECT

GENERIC MEETING	WMPO REQUEST FOR TPO ATTENDANCE	TPO RESPONSE	NNWSI REPRESENTATIVES
<ul style="list-style-type: none"> o Seismic/Tectonic o 8/20-21 o Washington, D.C. 	<ul style="list-style-type: none"> o LANL -- 7/21 o SAIC -- 7/21 o SNL -- 7/21 	<ul style="list-style-type: none"> o SAIC -- 7/16 o SNL -- 7/05 	<ul style="list-style-type: none"> o Syzmanski (WMPO) o Blanchard (WMPO) o Voegele (SAIC) * o
Subramanian (SNL)			
<ul style="list-style-type: none"> Retrievability Position o 7/31 o Washington 	<ul style="list-style-type: none"> o SNL -- 7/21 	<ul style="list-style-type: none"> o SNL -- 7/15 o SAIC -- 7/16 	<ul style="list-style-type: none"> o Neal (SNL) o Scully (SNL) o Flores (SNL) o Voegele (SAIC) * o Syzmanski (WMPO)
Subsystem Performance			
<ul style="list-style-type: none"> Allocation o 9 o Washington, D.C. 	<ul style="list-style-type: none"> o SNL -- 7/21 	<ul style="list-style-type: none"> o SNL -- 7/05 	<ul style="list-style-type: none"> o Bingham (SNL) *
EA Comment Response			
<ul style="list-style-type: none"> o 8-9 o Washington 	<ul style="list-style-type: none"> o SAIC -- 7/21 	<ul style="list-style-type: none"> o SAIC -- 7/16 	<ul style="list-style-type: none"> o Younker (SAIC) *
SCP Issue Resolution			
<ul style="list-style-type: none"> o 9-10 o Washington, D.C. 	<ul style="list-style-type: none"> o SAIC -- 7/21 	<ul style="list-style-type: none"> o SAIC -- 7/16 o SNL -- 7/05 	<ul style="list-style-type: none"> o Voegele (SAIC) o Jorgenson (SAIC) * o Stevens (SNL) o Tuebner (SAIC) o Richards (SNL)
Q-list methodology	No specific request	o SNL -- 7/05	
<ul style="list-style-type: none"> o 7/01 o Washington, D.C. 			
Generic ES Test Plans, Construction and Licensing	No specific request	<ul style="list-style-type: none"> o SNL -- 7/05 o SAIC -- 7/16 	<ul style="list-style-type: none"> o Tillerman (SNL) * o Fernandez (SNL) o Voegele (SAIC) o Syzmanski (WMPO) o Richards (SNL)
<ul style="list-style-type: none"> o 7/17-19 o Washington, D.C. 			
Generic Q.A. Meeting	No specific request	o SNL -- 7/05	
<ul style="list-style-type: none"> o 7-8 o Washington, D.C. 			



NNWSI MEETINGS	WMPD DUE-DATE FOR OBJECTIVES	AGENDA	OBJECTIVES	RESPONSE ON AGENDA	REFERENCES TO NRC
<u>Waste Package</u>	NRC: 7/01	NRC: 7/03	NRC: 7/01	NRC: (informal)	Sent on
o When -- 7/23-24					
o Where -- LLNL	LLNL: 7/11	LLNL: 6/11	LLNL: 5/21	LLNL: 6/18	7/03
o Lead -- L. Ballou (LLNL)					
o Status -- COMPLETE					
<u>E. S. Design</u>	NRC: 7/30	NRC: 8/13	NRC:	NRC:	Sent on
o When -- 8/27-28					
o Where: TBD					6/7
o Lead: Nelson (LLNL)	LANL: 7/01	LANL: 7/12	LANL: 7/16	LANL: 7/16	7/9
o Status: INCOMPLETE					
<u>E.S. Test Plan (See attached)</u>					
<u>U. Z. Hydrology and Geochemistry</u>	NRC: 8/26	NRC: 9/9	NRC:	NRC:	
o When -- 9/23-26					
o Where -- TBD					
o Lead -- NRC					
o Status -- INCOMPLETE					
<u>Performance Assessment Plan</u>	NRC: 9/03	NRC: 9/17	NRC:	NRC:	Due
o When -- 10/1-4					
o Where -- TBD	SNL: 7/30	SNL: 8/20	SNL:	SNL:	8/20
o Lead -- (SNL)					
o Status -- INCOMPLETE					

DRAFT 6 OF THE EPA STANDARD 40CFR191

o **ACRS COMMENTS**

- **STANDARD IS SERIOUSLY FLAWED AND SHOULD BE RELAXED BY A FACTOR OF 10**
- **CRITICAL OF NRC STAFF FOR CONCURRING IN DRAFT 6**
- **WILL ASK COMMISSION TO TAKE THEIR CONCERNS INTO ACCOUNT BEFORE THE COMMISSION COMMENTS ON THE STANDARD**

o **NRC COMMENTS**

- **STANDARD IS ACHIEVABLE AND IS COMPATIBLE WITH 10CFR60**
- **DOE MUST ACCOUNT FOR UNCERTAINTIES WHEN ASSESSING SITES AGAINST THE STANDARD**

o **DOE/HQ COMMENTS**

- **NO MAJOR ISSUES WITH EPA STANDARD**
- **RELAXING THE STANDARD WOULD NOT CHANGE DOE'S CURRENT SELECTION OF SITES**

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PROJECT

**SECRETARY OF ENERGY'S PRELIMINARY DETERMINATION
OF SITE SUITABILITY**

**114(F) OF NWPA: "_____THE SECRETARY SHALL CONSIDER AS
ALTERNATIVE SITES FOR THE FIRST REPOSITORY ____3 CANDIDATE
SITES WITH RESPECT TO WHICH (1) SITE CHARACTERIZATION HAS
BEEN COMPLETED UNDER SECTION 113; AND (2) THE SECRETARY
HAS MADE A PRELIMINARY DETERMINATION, THAT SUCH SITES ARE
SUITABLE FOR DEVELOPMENT AS REPOSITORIES CONSISTENT WITH
THE GUIDELINES PROMULGATED UNDER SECTION 112(A)."**

WHEN SHOULD THE PRELIMINARY DETERMINATION BE MADE BEFORE OR AFTER SITE CHARACTERIZATION?

- **NRC POSITION:** " THE COMMISSION AND DOE AGREED THAT THE PRELIMINARY DETERMINATION REQUIRED BY SECTION 114(F) OF THE NWPA SHOULD BE MADE AFTER THE COMPLETION OF SITE CHARACTERIZATION AND NOT AT THE TIME OF SITE NOMINATION AND RECOMMENDATION."
(49FR28139, JULY 10, 1984)
- **DOE POSITION:** ACCORDING TO DOE'S DRAFT PROJECT DECISION SCHEDULE (JANUARY, 1985), THE PRELIMINARY DETERMINATION WILL BE MADE AFTER SITES ARE SELECTED FOR CHARACTERIZATION.
- **SENATE COMMITTEE ON ENERGY AND NATURAL RESOURCES POSITION:**
" REQUIRING THAT THE PRELIMINARY DETERMINATION BE MADE AFTER THE COMPLETION OF SITE CHARACTERIZATION IS AT ODDS WITH THE LANGUAGE AND INTENT OF THE ACT."
(JUNE 25, 1985 LETTER FROM SENATORS JOHNSTON, SIMPSON McCURE AND DOMENICI TO SECRETARY JOHN HERRINGTON)

IMPORTANCE OF COUPLED PROCESSES

IN NNWSI ASSESSMENTS

TOWARDS A POSITION PAPER

C. F. Keller

Los Alamos National Laboratory

MOTIVATION

The possibilities of thermal chemical, hydrodynamic and mechanical processes interacting in a manner that would be deleterious to waste containment is a serious concern to the DOE and NRC.

A systematic evaluation of such coupled processes needs to be made to evaluate which are important.

MOST IMPORTANT CURRANT CONCERNS:

Thermo-Hydro-Mechanical

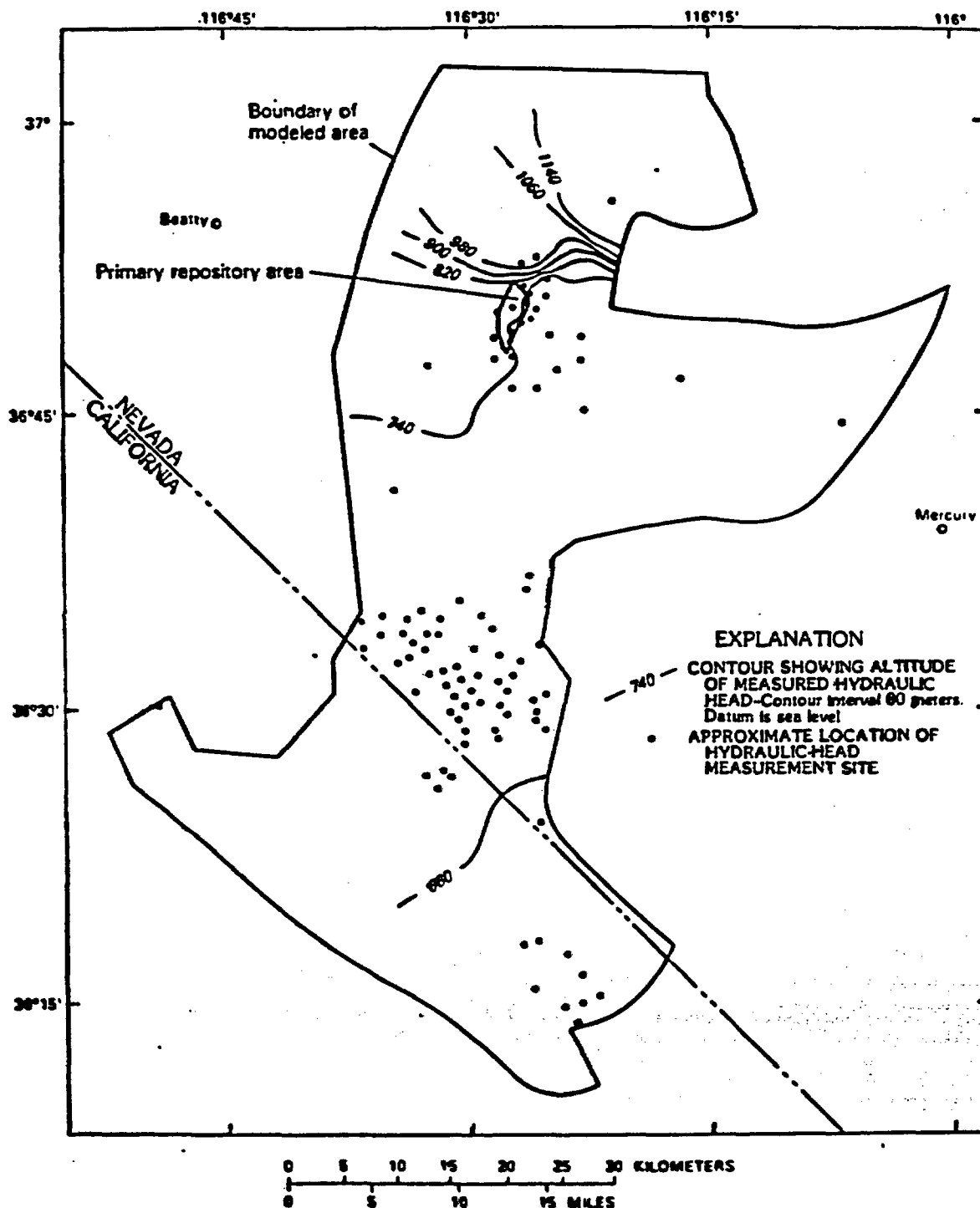
If repository heating of host rock induces change in pore pressure in disturbed zone, will Yucca Mountain go so far into tension as to open additional flow paths?

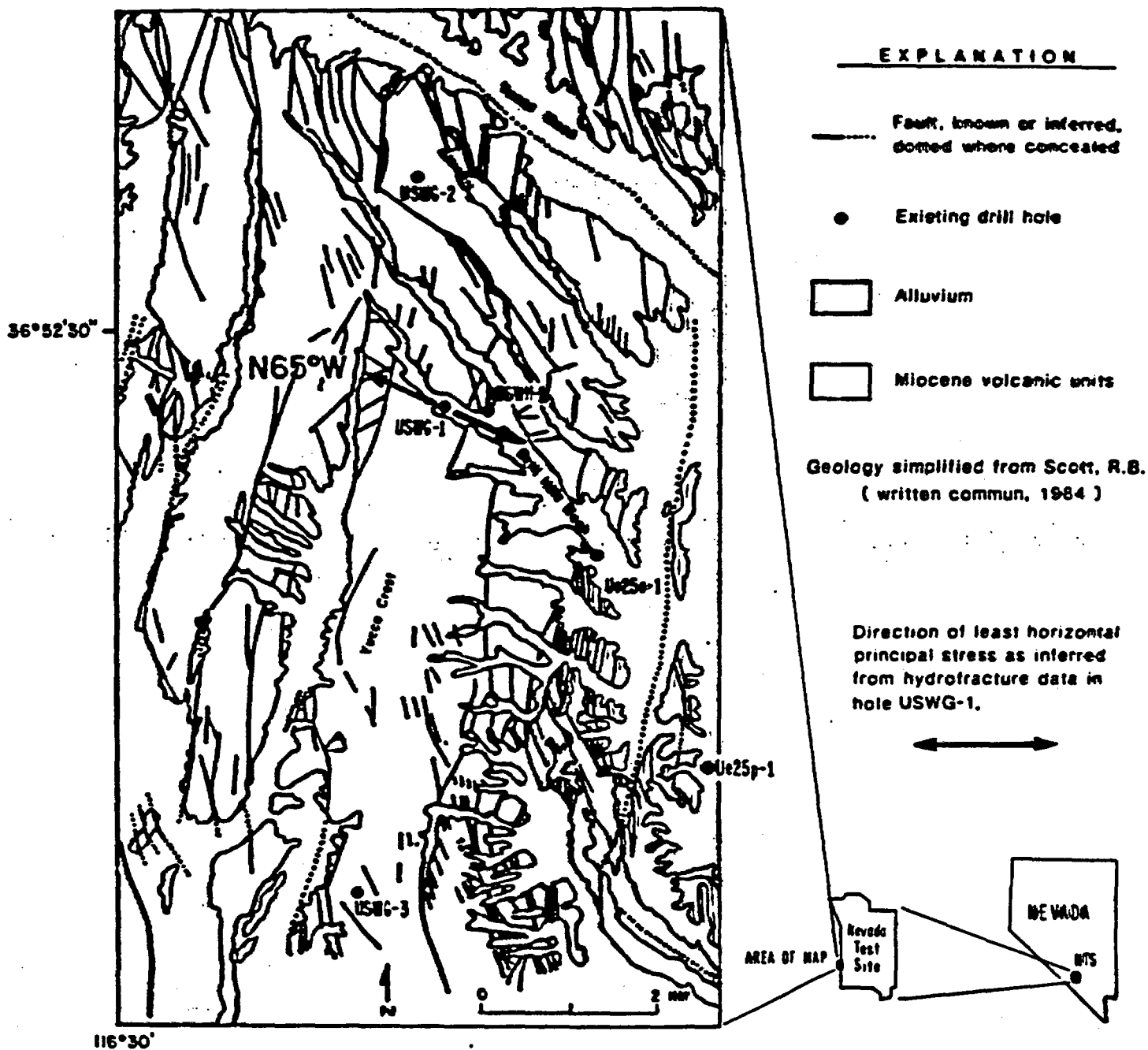
Will such flow paths create a positive feedback loop putting mountain further into tension?

Hydro-Mechanical

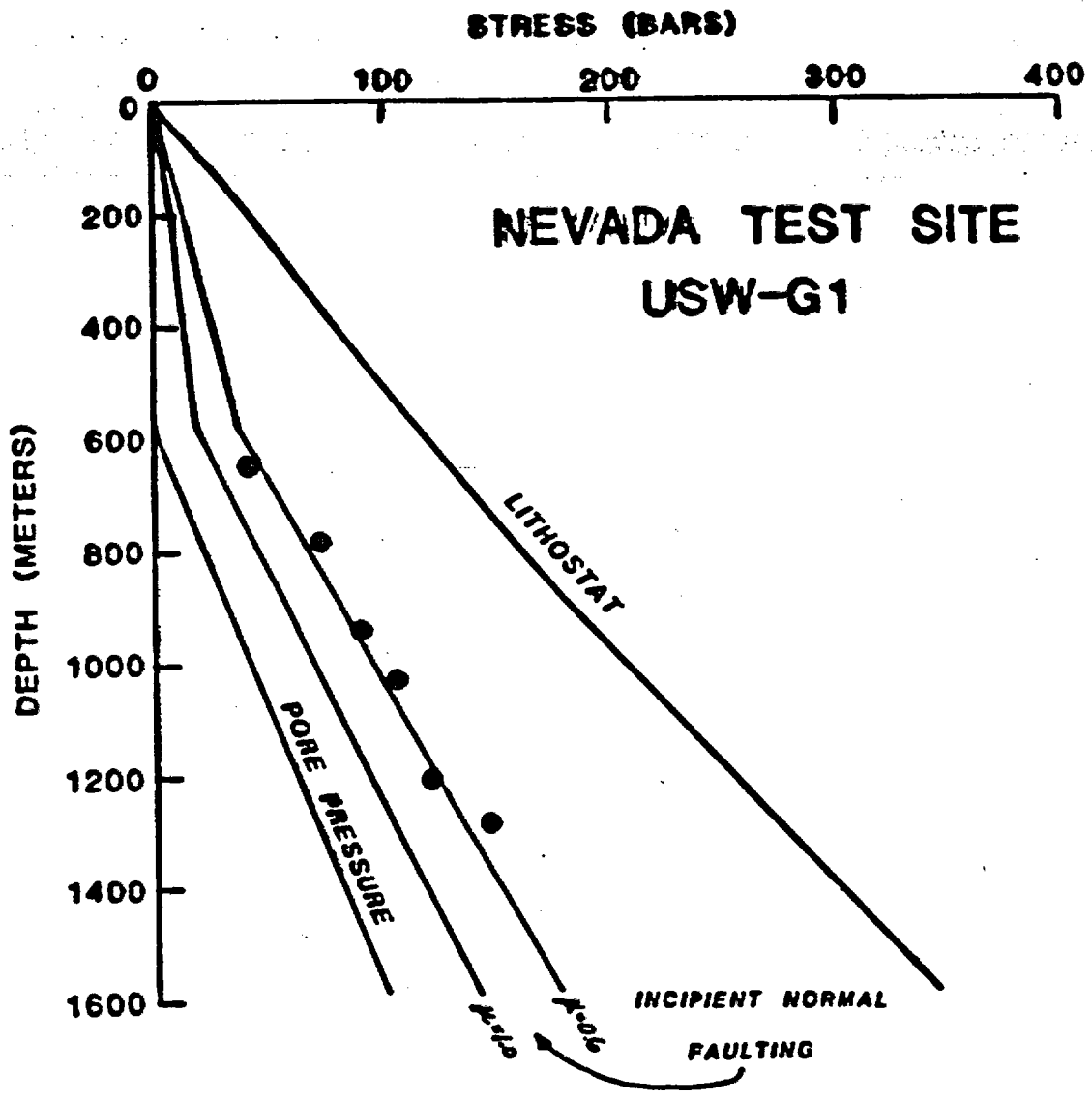
What interactions could occur between the high water table north of the repository and induced stress states in the rock?

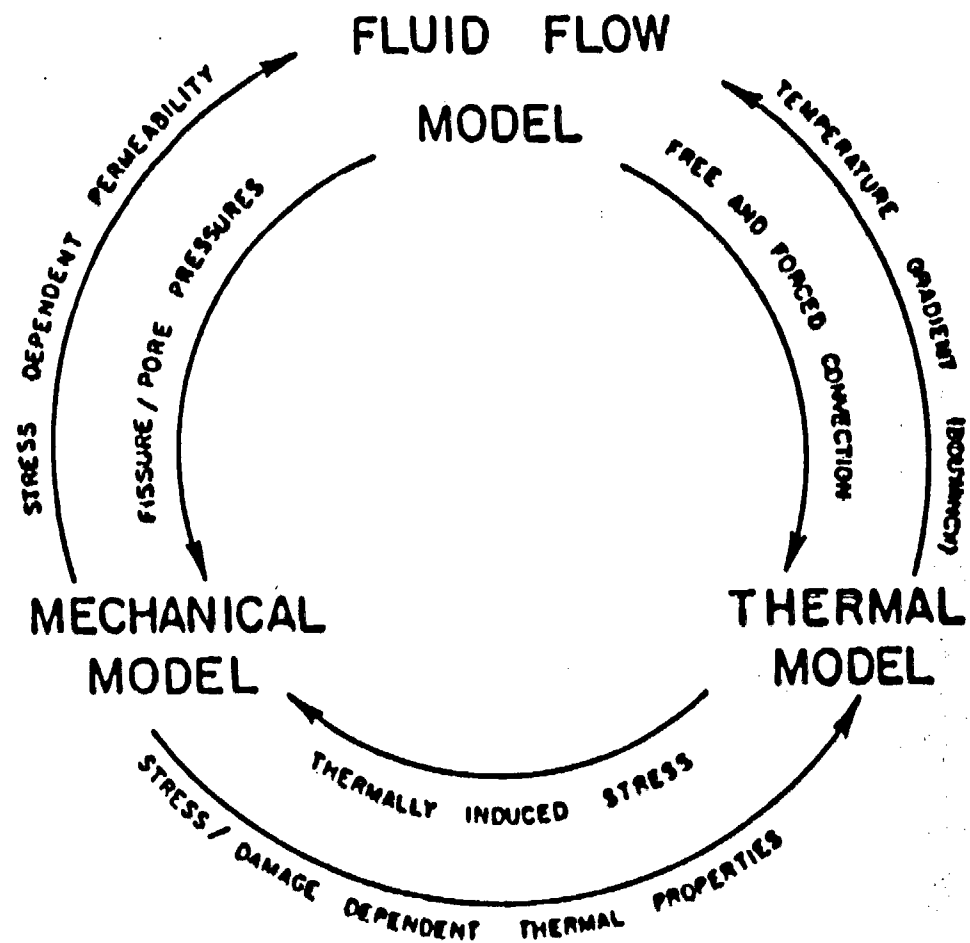
Could a change in stress cause the water stored in that volume to move across the repository as a large pulse?

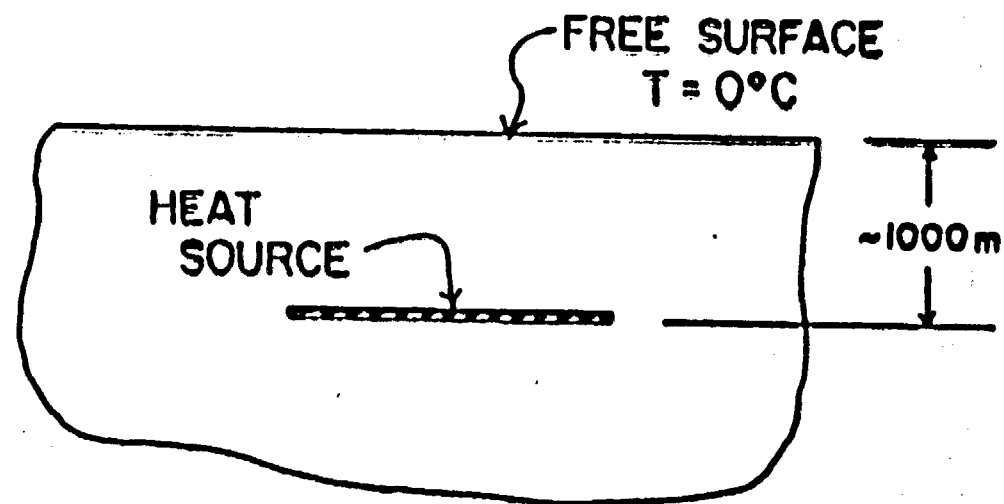


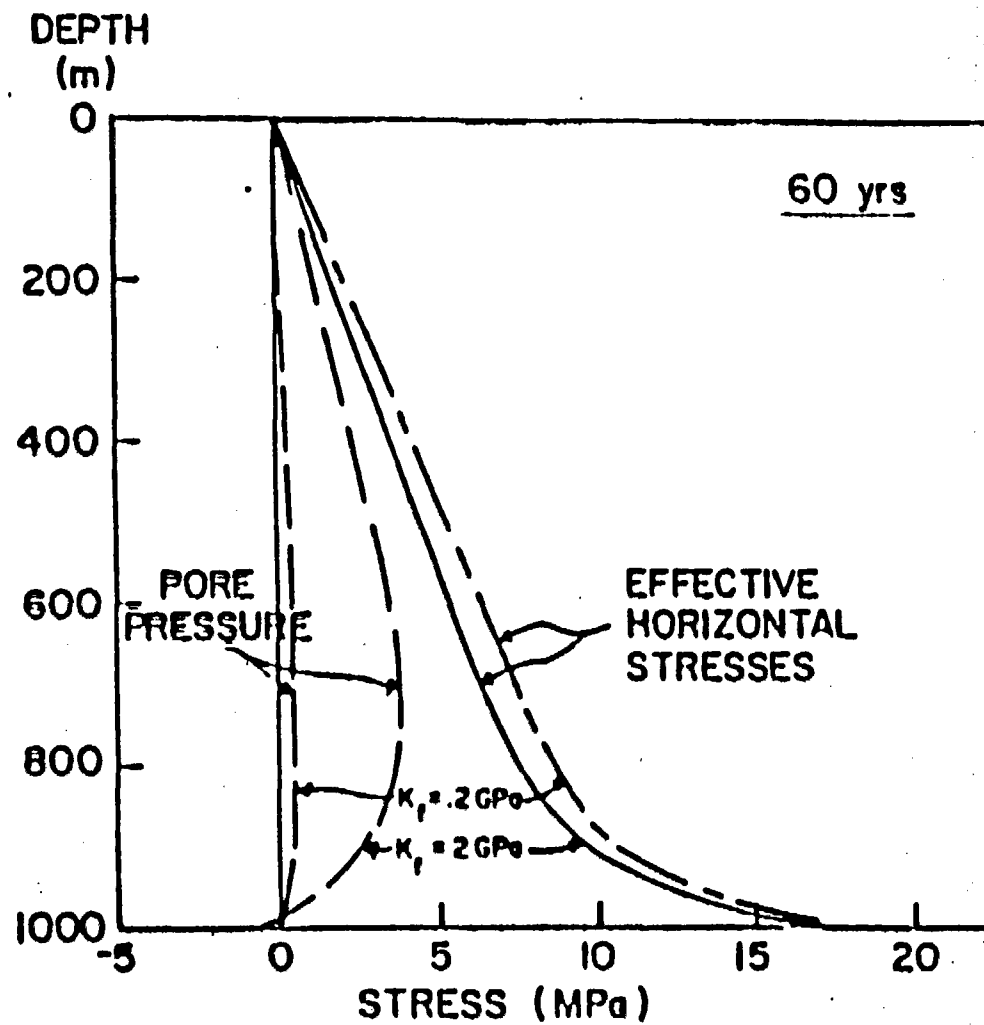


Geologic map of Yucca Mountain area.









RESOURCES:

Gail Cederberg's Paper

"Report on NNWSI Efforts in Coupled Processes "

Other untapped expertise

At the Laboratories

At other institutions

e.g. Roger Hart, Univ. Minn.

SUMMARY OF INVESTIGATIONS INTO COUPLED PROCESSES (CONTINUED)

<u>PROCESS</u>	<u>METHOD OF INVESTIGATION</u>	<u>PI/ORGAN.</u>
<u>Thermomechanical</u>		
Rock Deformation, Including Fracture Closure Due to Temperature Effects (heating and cooling phases)	Field Experiment: ESTP; Waste Package Environment Tests; Reduced-Scale Heater Tests	Yow/LLNL
Effects of Thermal Stresses on Fracture Apertures	Laboratory Experiments	Nimick/SNL
Effects of Thermomechanical Properties on Rock Mass Properties	Numerical Modeling; FEM using Field and Laboratory Data	Bauer SNL
Effects of Temperature and Pressure on Mechanical Tuff Properties	Laboratory Experiments	Nimick/SNL
Effects of Thermal Loading on Underground Facility and Design	Numerical Modeling	Manure/ SNL
<u>Hydrochemical</u>		
Particle Transport (Colloids)	Numerical Modeling and Laboratory Column Experiments	Travis and Nuttall, Rundberg/ LANL
Variations in Geochemical Transport Due to Changes in Chemical Parameters	Numerical Modeling	Cederberg/ LANL
Effects on Transport Due to Co-Precipitation Reactions	Numerical Modeling	Cederberg/ LANL
Effect of Microbiological Activity on Groundwater Composition and Transport	Laboratory Experiments	Ogord/ LANL
In Situ Retardation of Noneroding Waste Elements, Colloids, and Particulates in the Saturated Zone	Field Experiments; Well-to-Well Pumping Tests	Ogord/ LANL
Chemical-Flow Coupling	Laboratory Experiments; Solid Tuff Columns, Rock Columns, Fractured Tuff Columns	Rundberg/ LANL

DRAFT

SUMMARY OF INVESTIGATIONS INTO COUPLED PROCESSES WITH
REGARD TO A VUCCA MOUNTAIN REPOSITORY

Gail A. Cederberg

Los Alamos National Laboratory
ESS-5, Los Alamos, NM 87545
July 11, 1985

<u>PROCESS</u>	<u>METHOD OF INVESTIGATION</u>	<u>PI/ORGAN.</u>
<u>Thermochemical</u>		
Chemistry of Fluid Flow in Near Field as a Function of Temperature (heating and cooling phases)	Field Experiment; ESTP; Waste Package Environment Tests; Reduced-Scale Heater Tests	Yew/LLNL
Rock Mineralogy Changes Due to Temperature (heating and cooling) Effects	Field Experiment; ESTP; Waste Package Environment Tests; Reduced-Scale Heater Tests	Yew/LLNL
Zeolite Stability	Laboratory Experiments	Vaniman/ LANL
Stability of Glass as a Function of Temperature	Laboratory Experiments	Vaniman/ LANL
Effect of Temperature on Mineral Dissolution and Precipitation	Laboratory Experiments	Vaniman/ LANL
Sorption Coefficients as a Function of Temperature	Laboratory Experiments	Thomas/ LANL
<u>Hydrothermal</u>		
Flow of Water, Steam, and Air as a Function of Temperature (heating and cooling phases)	Field Experiment; ESTP; Waste Package Environment Tests; Reduced-Scale Heater Tests	Yew/LLNL
Permeability as a Function of Temperature	Numerical Modeling	Hayden/SNL

IMMEDIATE GOAL:

POSTITION PAPER AT BERKELEY COUPLED PROCESSES MEETING

Position will be based on Cederberg's Table from her report and on work of Task Force set up by Szymanski.

Bill McNabb - SAIC

LIMS/LIMP

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S YSTEM

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SCOPE

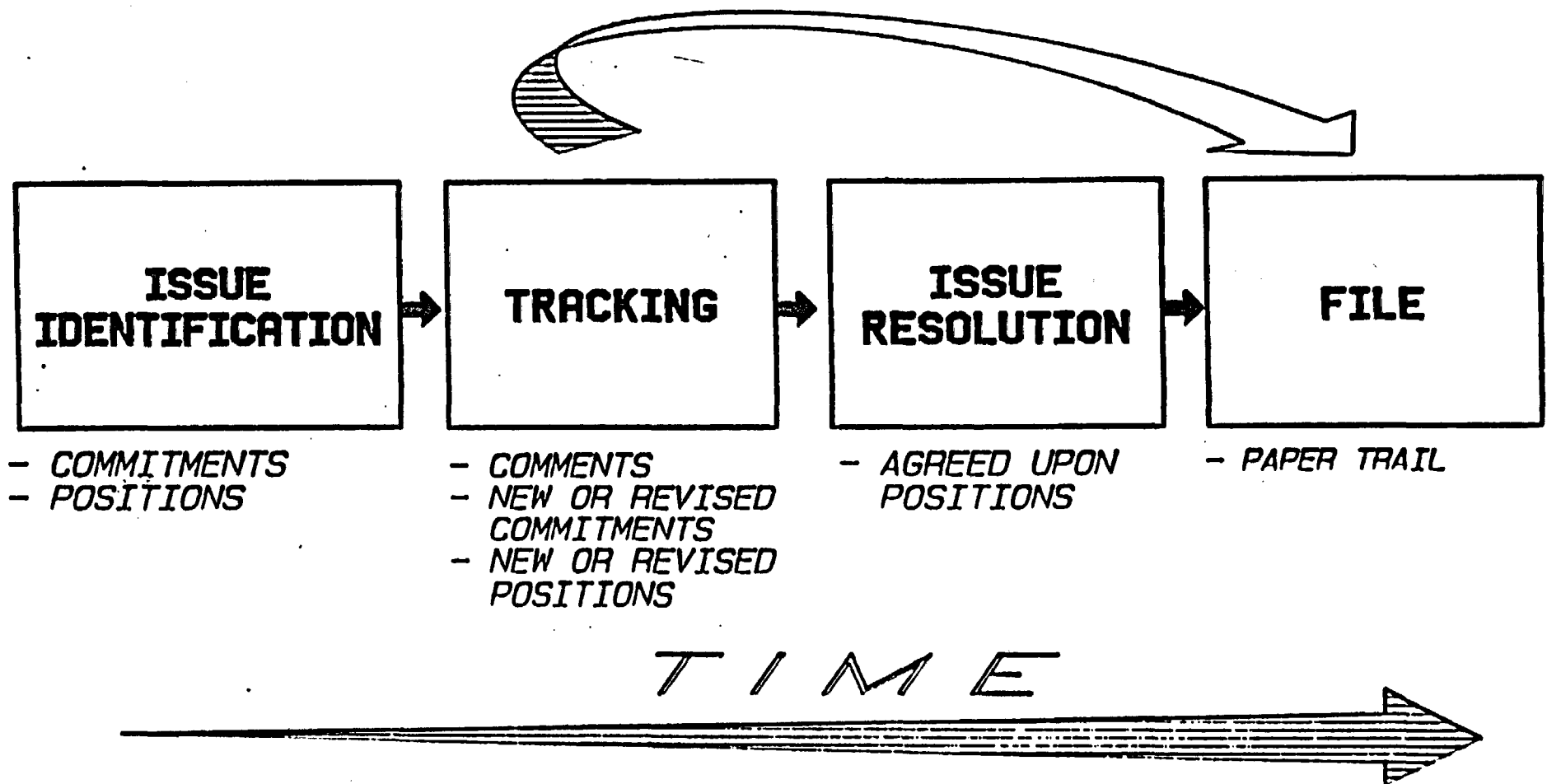
THE ELECTRONIC STORAGE OF INFORMATION THAT...

**"EITHER DIRECTLY SUPPORT LICENSING (QA LEVEL 1) OR
RELATE TO REGULATORY ACTIVITIES ASSOCIATED WITH
LICENSING"**

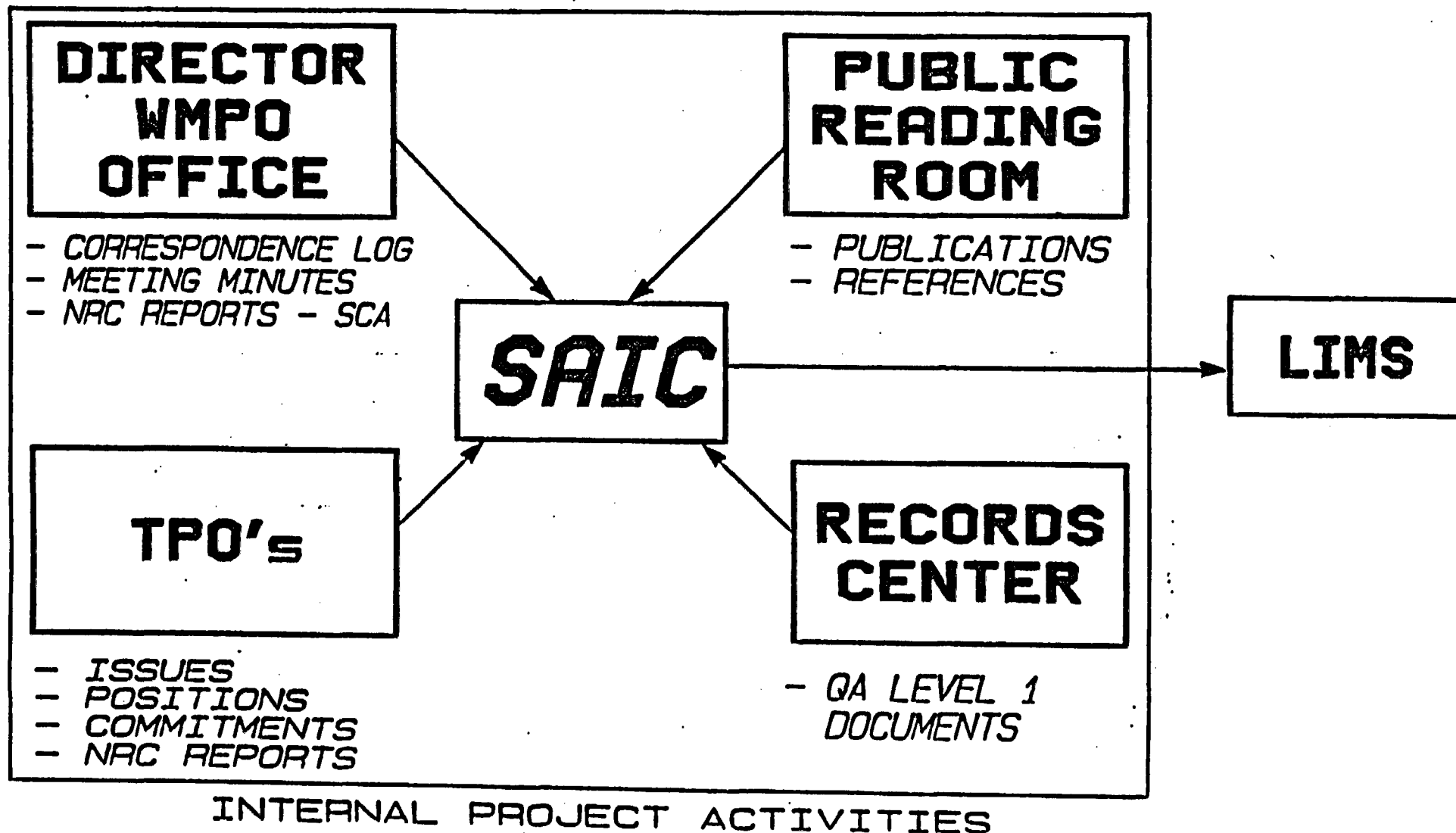
PURPOSES

- (1) PROVIDE A FILE WHICH DOCUMENTS FOR THE PUBLIC RECORD THE PROCESS OF DECISION MAKING IN THE RESOLUTION OF ISSUES FOR LICENSING**
- (2) PROVIDE AT A POINT IN TIME THE SAME FILE TO EVERYONE DOCUMENTING THE STATUS OF SUCH LICENSING**
- (3) BE A RESOURCE FOR SEARCHING, SORTING, AND RETRIEVING INFORMATION IN RESPONSE TO OUTSIDE REQUESTS DURING THE REGULATORY PROCESS (PRE-LICENSING, DISCOVERY, PRE-HEARING AND HEARING)**
- (4) BE A TOOL TO ASSIST WMPO IN MANAGING THE REGULATORY PROCESS (BOTH PRE-LICENSING AND LICENSING)**

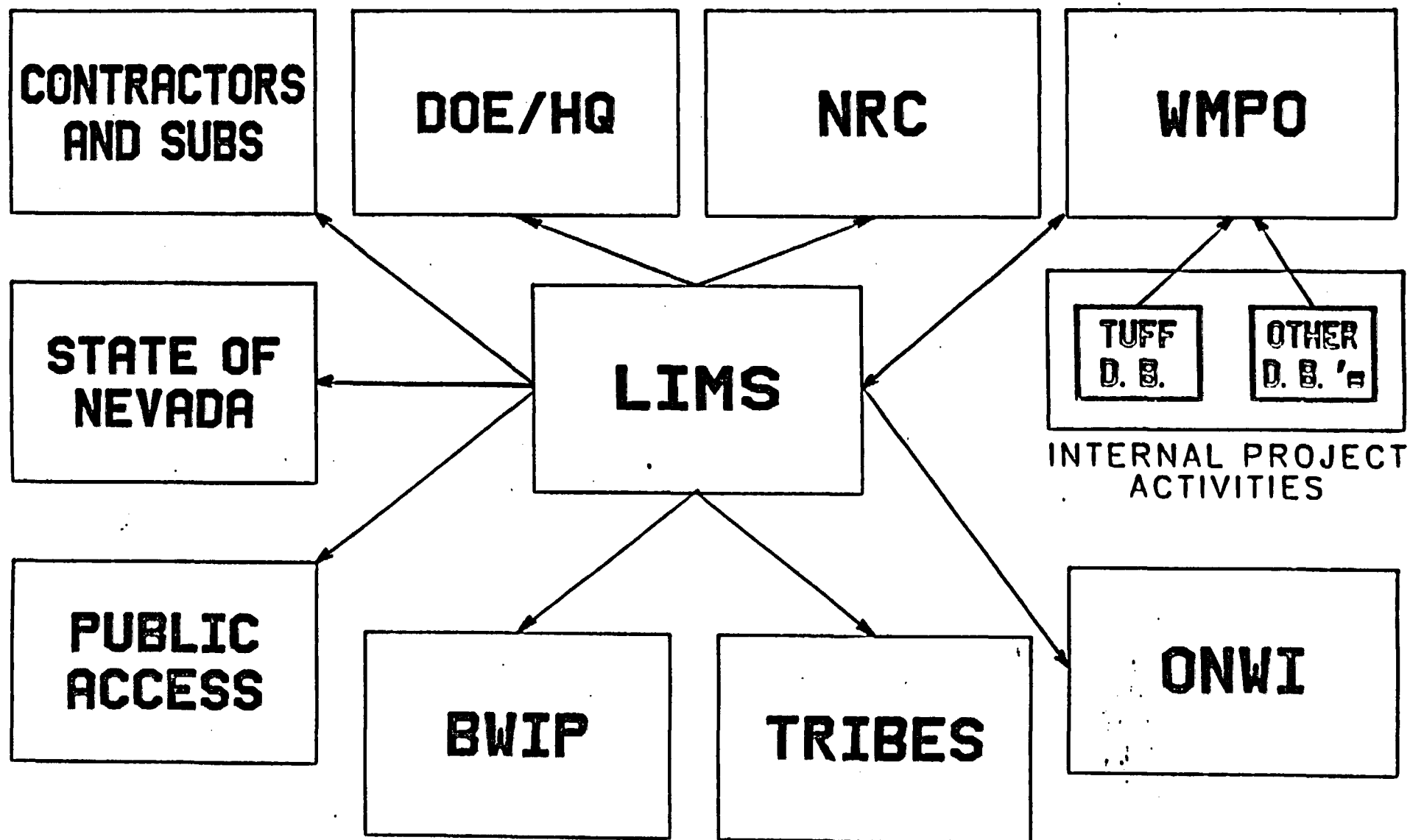
OVERALL LIMS CONCEPT



EXAMPLE OF NNWSI STRUCTURE



EXAMPLE OF INFORMATION FLOW



PLANNED ACTIVITIES - NEAR TERM

- (1) VISIT ONWI AND BWIP TO OBSERVE SYSTEMS IN OPERATION**
- (2) REQUEST SPECIFIC INFORMATION ON EXISTING PLANNED INFORMATION MANAGEMENT SYSTEMS IN ORDER TO IDENTIFY WHAT CURRENTLY EXISTS**
- (3) EVALUATE SYSTEM CONCEPTS IN ORDER TO SELECT OPTIONS OF MOST VALUE TO NNWSI, E.G.,**
 - (a) FULL TEXT VS. INDEXED INPUT, STORAGE SEARCHING, AND RETRIEVAL**
 - (b) LEVEL OF NUMERICAL DATA TO INCLUDE IN PUBLICLY AVAILABLE SYSTEM**
 - (c) AMOUNT OF CONSISTENCY WITH DOE/HQ AND OTHER (DEVELOPED) SYSTEMS**
- (4) VISIT PROJECT PARTICIPANTS IN ORDER TO:**
 - (a) EXPLAIN LIMS CONCEPT TO STAFF**
 - (b) GET STAFF INPUT AS TO THEIR NEEDS (PRELIMINARY REQUIREMENTS DEFINITION)**
 - (c) GET BETTER UNDERSTANDING OF HOW INFORMATION FLOWS WITHIN THE PROJECT**

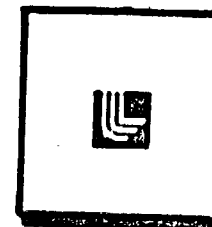
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**WVCC
MOUNTAIN**

DEVELOPMENT AND APPLICATION OF EQ3/6



PRESENTATION TO THE JULY PM-TPO MEETING OF THE NNWSI

**J. DELANY
K. JACKSON
L. RAMSPOTT
T. WOLERY**

**JULY 24, 1985
LAS VEGAS**

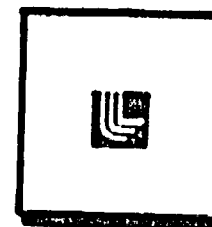
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HEALTH**

DEVELOPMENT AND APPLICATION OF EQ3/6



	TIME: (MINS.)
● INTRODUCTION - LARRY RAMSPOTT	15
● DEVELOPMENT - TOM WOLERY	30
● GENERAL APPLICATIONS - KEN JACKSON	25
● WASTE PACKAGE APPLICATIONS - JOAN DELANY	50

OCRWM

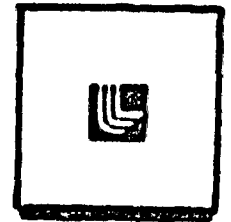
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YIPER PLANT

DEVELOPMENT AND APPLICATION OF EQ3/6

INTRODUCTION



- HISTORY OF EQ3/6
- PRESENT FUNDING STRUCTURE
- EQ3/6 PROGRAMMATIC ORGANIZATION
- EXTENT OF ACCEPTANCE AND USE OF EQ3/6 OUTSIDE NNWSI (AND OCRWM PROGRAM)

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EQ3/6: HISTORY OF SUPPORT



**1975-77 T. J. WOLERY PH.D. DISSERTATION, NORTHWESTERN UNIVERSITY
(INTERACTIONS OF SEA WATER WITH BASALT IN MID-OCEAN RIDGE
HYDROTHERMAL SYSTEMS)**

1978-80 WOLERY AT LLNL. DEVELOPMENT SPONSORED BY

**DOE: OFFICE OF BASIC ENERGY SCIENCES
GEOTHERMAL ENERGY PROGRAM**

NRC: WASTE MANAGEMENT PROGRAM

1980-82 DOE THROUGH PNL'S WISAP PROGRAM

1983-85 DOE THROUGH ONWI (SRPO) AND NNWSI

1986 NNWSI, SRPO, BWIP

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Nuclear Waste

EQ3/6: CURRENT FUNDING ARRANGEMENTS FOR DEVELOPMENT
AND MAINTENANCE

FY 1985

NNWSI - 530K

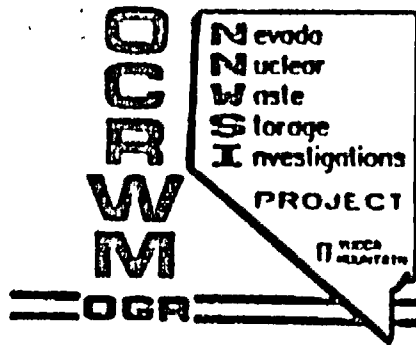
ONWI - 300K

FY 1986

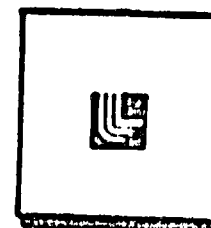
NNWSI - 695K

ONWI - 350K

BWIP - 70K



INTEREST IN OF USE OF EQ3/6 IS WIDESPREAD



- THE NUMBER OF ACTUAL USERS OUTSIDE LLNL IS ESTIMATED TO BE IN THE RANGE 70-120.
- THE MAILING LIST NOW CONTAINS 225 ENTRIES.
 - 62 PEOPLE AT 46 UNIVERSITIES AND INSTITUTES (43/28 U.S., 18/19 FOREIGN).
 - 21 PEOPLE AT 6 D.O.E. NATIONAL LABORATORIES (INCLUDING LLNL) PLUS 6 AT PNL AND 7 AT USGS.
 - 27 PEOPLE AT 22 FOREIGN NON-UNIVERSITY RESEARCH ORGANIZATIONS, REPRESENTING 12 COUNTRIES.
 - 13 PEOPLE AT 9 U.S. OIL COMPANIES.

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EQ3/6: AN APPLICATIONS BIBLIOGRAPHY



FORMATION OF ORE DEPOSITS:

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- G. GARVEN, THE ROLE OF GROUNDWATER FLOW IN THE GENESIS OF STRATABOUND ORE DEPOSITS: A QUANTITATIVE ANALYSIS, PH.D. THESIS, UNIVERSITY OF BRITISH COLUMBIA, VANCOUVER, BRITISH COLUMBIA, 1982.
- D. SVERJENSKY, "OIL FIELD BRINES AS ORE-FORMING SOLUTIONS", ECON. GEOL. 79, 23-27 (1984).
- D. JANECKY AND W. E. SEYFRIED, JR., "FORMATION OF MASSIVE SULFIDE DEPOSITS ON OCEANIC RIDGE CRESTS: INCREMENTAL REACTION MODELS FOR MIXING BETWEEN HYDROTHERMAL SOLUTIONS AND SEAWATER," GEOCHEMICA ET COSMOCHIMICA ACTA, VOL. 48, PP. 2723-2738.

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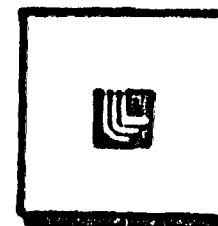
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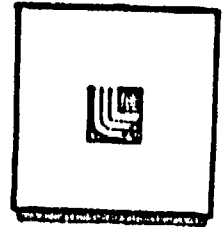
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EQ3/6 STATUS AND DEVELOPMENT - T.J. WOLERY



- WHAT EQ3/6 IS.
- IMPORTANT ASPECTS OF AND ISSUES PERTAINING TO GEOCHEMICAL MODELING.
- RECENT DEVELOPMENT.
- FUTURE WORK.

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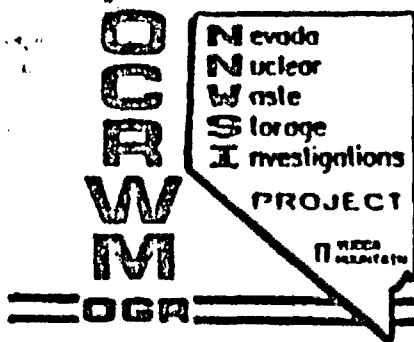
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EQ3/6 IS AN INTEGRATED SOFTWARE PACKAGE



- PERMITS GEOCHEMICAL CALCULATIONS IN AQUEOUS SYSTEMS OVER THE TEMPERATURE RANGE 0-300°C.
- CONSISTS OF TWO MAIN CODES, EQ3NR AND EQ6.
- CONTAINS A HANDFUL OF MINOR CODES FOR MANAGEMENT OF THERMODYNAMIC DATA BASES.
- ALSO CONSISTS OF SUPPORTING DATA FILES, INCLUDING A MAJOR TWO-TIER THERMODYNAMIC DATA BASE.
- IS VERY STATE OF THE ART.



THE EQ3NR CODE IS A "SPECIATION-SOLUBILITY" CODE



- COMPUTES A THERMODYNAMIC MODEL OF THE STATE OF AN AQUEOUS SOLUTION, GIVEN THERMODYNAMIC DATA AND ANALYTICAL DATA. THE LATTER MOSTLY CONSIST OF "TOTAL" CONCENTRATIONS AND PH.
- VARYING AMOUNTS OF DISEQUILIBRIUM CAN BE ASSUMED AT THE COST OF MORE SPECIFIC INFORMATION ABOUT THE PARTICULAR AQUEOUS SOLUTION BEING MODELED; E.G., IF $\text{Fe}^{2+}/\text{Fe}^{3+}$ ARE TO BE ASSUMED NOT CONTROLLED BY EH, THEN Fe^{2+} AND Fe^{3+} MUST BE MEASURED SEPARATELY, NOT JUST AS "TOTAL" FE.

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EQ3NR CODE (CONT.)



-
- CALCULATES VALUES OF ACTIVITY COEFFICIENTS OF AQUEOUS SPECIES (REQUIRED TO OBTAIN ITEMS BELOW).
 - CALCULATES THE EXTENT OF FORMATION OF ION PAIRS AND COMPLEXES.
 - CALCULATES SATURATION INDICES FOR SOLIDS FROM THE WATER COMPOSITION; ALTERNATIVELY, CAN CALCULATE SOLUBILITIES FOR SELECTED SOLIDS IN SOLUTIONS WHOSE COMPOSITIONS ARE OTHERWISE SPECIFIED.
 - CALCULATES ELECTRICAL IMBALANCE OF THE ANALYSIS.
 - ALTERNATIVELY, ADJUSTS A SELECTED INPUT CONCENTRATION OR THE PH TO ACHIEVE ELECTRICAL BALANCE.

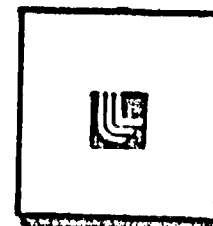
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THE EQ6 CODE IS A "REACTION-PATH" CODE



- ① COMPUTES A THERMODYNAMIC/KINETIC MODELS OF THE REACTION BETWEEN AN AQUEOUS SOLUTION AND SPECIFIED SOLIDS. CAN ALSO DEAL WITH TEMPERATURE CHANGES AND FLUID MIXING.
- ② THE MODEL OF THE INITIAL AQUEOUS SOLUTION COMES FROM EQ3NR.
- ③ THE CODE PREDICTS WHAT NEW PHASES FORM, SUBJECT TO USER GUIDANCE.
- ④ IT ALSO PREDICTS THE EVOLUTION OF THE AQUEOUS SOLUTION COMPOSITION.

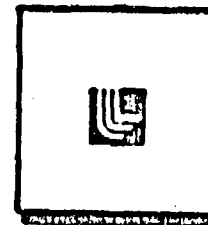
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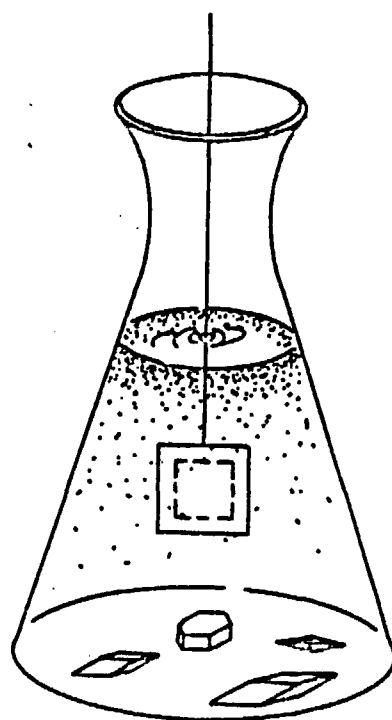
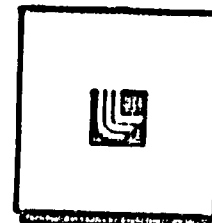
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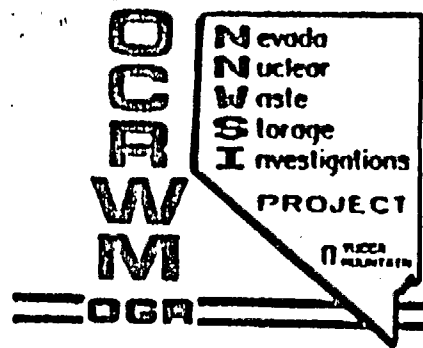
EQ6 CODE (CONT.)



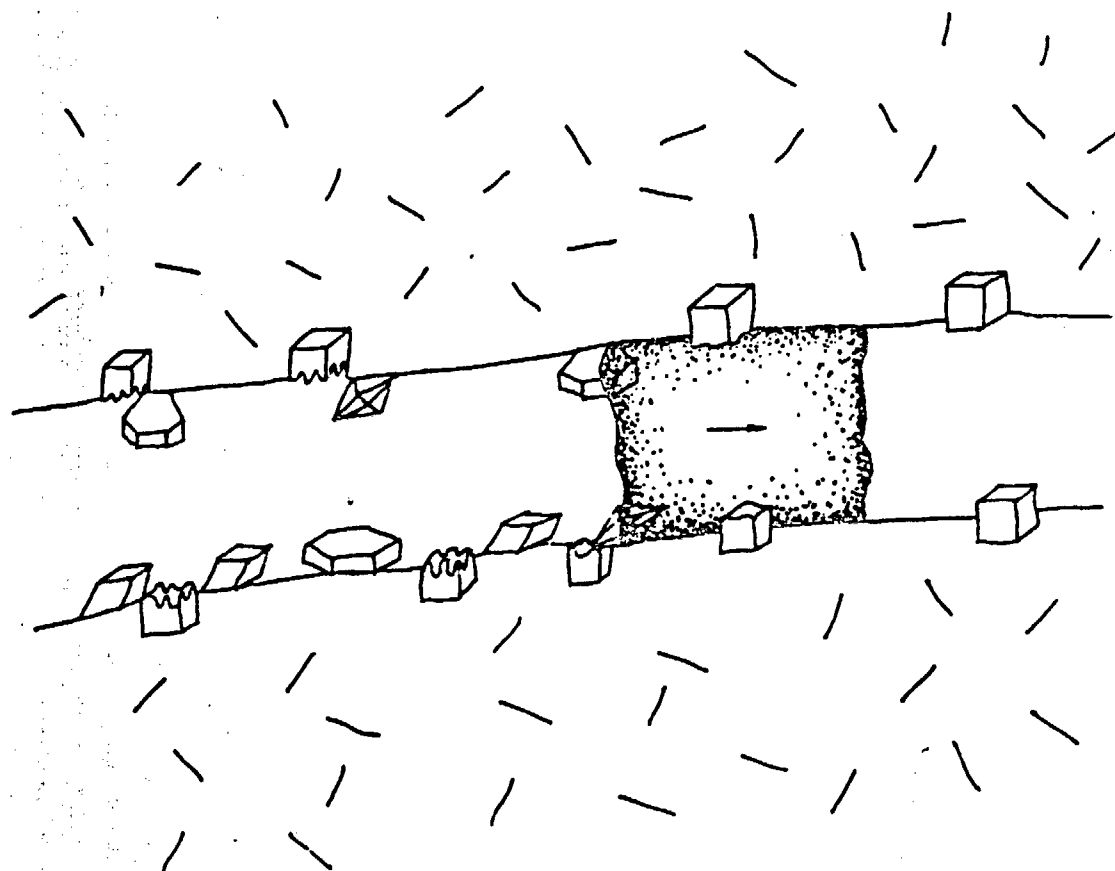
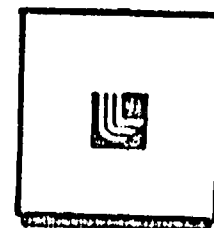
- ① EQ6 OPERATES IN MORE THAN ONE PHYSICAL MODE:
 - ① SIMPLE CLOSED SYSTEM (E.G., DICKSON AUTOCLAVE)
 - ① SYSTEM OPEN TO GASES (FIXED FUGACITY MODE)
 - ① PSEUDO-1-DIMENSIONAL FLOW THROUGH MODE, FOLLOWS THE EVOLUTION OF A PACKET OF MOVING WATER.
- ① WE MAY WANT TO ADD IN THE FUTURE:
 - ① PSEUDO-1-DIMENSIONAL FLOW THROUGH MODE, FOLLOWING CHEMICAL EVOLUTION AT A FIXED LOCATION (LEACHING CELL MODE).
 - ① FULLY 1-DIMENSIONAL FLOW THROUGH MODE.

EQ6 - CLOSED SYSTEM MODE





EQ6 - FLOW THROUGH MODE FOLLOWING THE
EVOLUTION OF A SINGLE PACKET OF WATER:



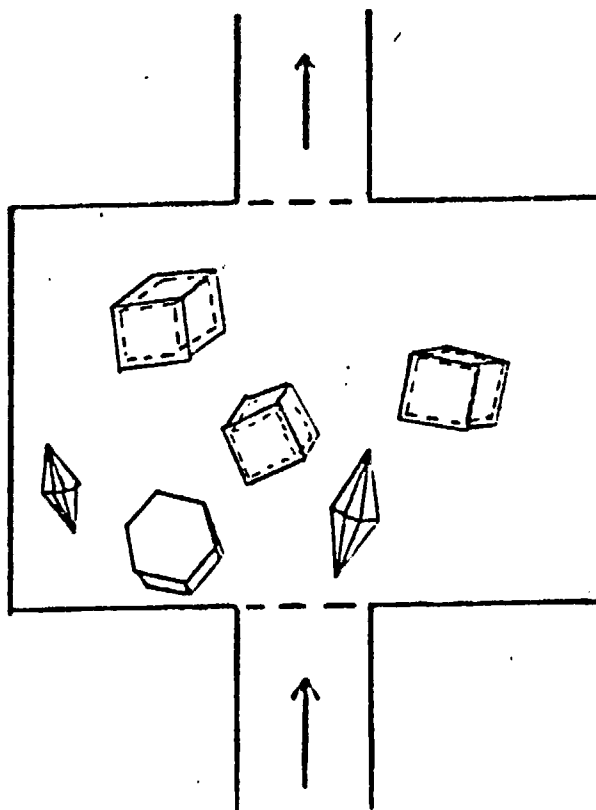
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FLOW THROUGH LEACHING CELL MODE
(NOT CURRENTLY IN EQ6)

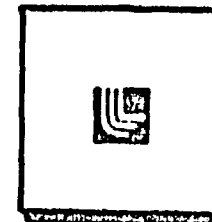


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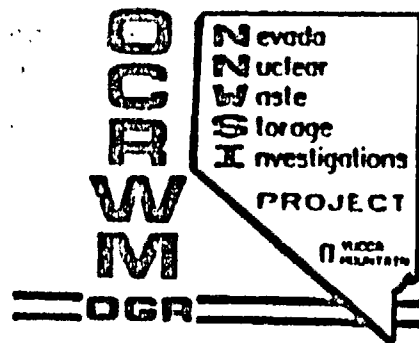
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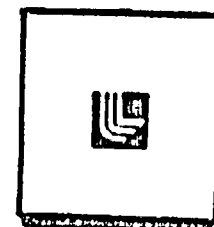
EQ3/6 HAS A TWO-TIER THERMODYNAMIC DATA BASE



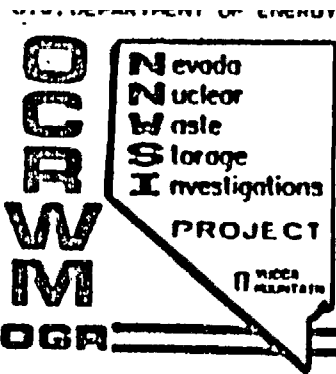
- AN OPERATIONAL DATA BASE TO SUPPORT EQ3/6 CALCULATIONS (DATA0). IT INCLUDES SOURCE TRACEBACK INFORMATION, BUT NOT DETAILED REFERENCES.
- A LARGER, UNDERLYING DATA BASE FROM WHICH SELECTED DATA ARE DRAWN (MDA). THE DATA HERE ARE MOSTLY IN DIFFERENT FORM THAN IN DATA0. FULL REFERENCES ARE GIVEN. INFORMATION ON ALTERNATE DATA VALUES, DISCREDITED DATA, AND DISCREDITED SPECIES IS INCLUDED HERE.
- A LARGE SUBSET OF DATA, MOSTLY FOR ALUMINOSILICATES, IS ALSO DRAWN FROM SUPCRT, A DATA BASE PRODUCED AND MAINTAINED AT THE UNIVERSITY OF CALIFORNIA AT BERKELEY.



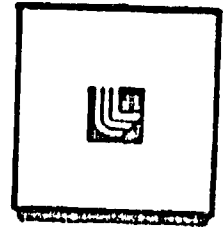
THE MCRT CODE PROCESSES DATA FROM MDA



- ① MCRT = MINERAL AND CHEMICAL REACTION THERMODYNAMICS.
- ① CONSTRUCTS THERMODYNAMIC DATA FOR REACTIONS FROM DATA FOR INDIVIDUAL SPECIES.
- ① PERFORMS TEMPERATURE EXTRAPOLATIONS, USING ANY OF SEVERAL ALGORITHMS.
- ① CARRIES OUT SEVERAL KINDS OF CONSISTENCY TESTS AND FLAGS ANY DETECTED ERRORS.
- ① WRITES DATA BLOCKS FOR INSERTION OR REPLACEMENT INTO DATA0, THE EQ3/6 OPERATIONAL DATA BASE.



EQUILIBRIUM HAS BEEN ABUSED IN GEOCHEMICAL MODELING



- ① MOST GEOCHEMICAL CODES HAVE BEEN LARGELY BASED ON EQUILIBRIUM ASSUMPTIONS.
- ① ASSUMING EQUILIBRIUM MEANS THAT FEWER MEASUREMENTS ARE NEEDED ON THE PROBLEM AT HAND; MOSTLY, ONE REQUIRES THERMODYNAMIC DATA.
- ① UNFORTUNATELY, MOST REAL SYSTEMS DON'T FOLLOW EQUILIBRIUM SO CLOSELY OR SO COMPLETELY.
- ① OFTEN, THE FIELD GIVES RESULTS CLOSER TO EQUILIBRIUM THAN DOES THE LABORATORY.
- ① KINETICS IS STILL A RELATIVELY NEW THING IN GEOCHEMISTRY.

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GEOCHEMICAL CALCULATIONS REQUIRE ESTIMATION OF THERMODYNAMIC ACTIVITIES



• FOR PURE SOLIDS, $A_S = 1$. NO PROBLEM HERE.

• FOR COMPONENTS OF SOLID SOLUTIONS, $A_J = X_J \lambda_J$

• X_J = MOLE FRACTION, λ_J = ACTIVITY COEFFICIENT.

• STATE OF THE ART WORK REQUIRED HERE.

• FOR AQUEOUS SPECIES, $A_I = M_I \gamma_I$

• M_I = MOLAL CONCENTRATION, γ_I = ACTIVITY COEFFICIENT.

• ADVANCED THEORIES REQUIRED FOR BRINE SOLUTIONS.

ONWI IS SUPPORTING LLNL DEVELOPMENT OF AN
ADVANCED THEORY FOR ITS WASTE MANAGEMENT PROBLEMS.

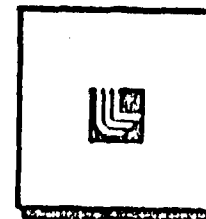
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EQ3/6 WORK IS EXTENDING THE STATE OF THE ART



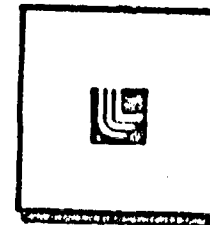
- HOW FAR CAN GEOCHEMICAL MODELING BE PUSHED IN SUPPORT OF WASTE MANAGEMENT ACTIVITIES? IT IS NECESSARY TO FIND OUT BY DOING, MAKING A REASONABLE BALANCE BETWEEN TRADE-OFFS.
- WE MUST BE THE LEADING EXPERTS AT LICENSING TIME, PARTICULARLY WHERE EXTRAPOLATIVE CALCULATIONS ARE CONCERNED.
- WE MUST BE AWARE OF DEVELOPMENTS ELSEWHERE IN WASTE MANAGEMENT AND IN THE OUTSIDE GEOCHEMISTRY AND CHEMISTRY COMMUNITIES THAT IMPACT WHAT WE ARE TRYING TO ACCOMPLISH, AND RESPOND APPROPRIATELY.

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EQ3/6 REQUIRES A SMART USER



- ① A PROBLEM GIVEN IN GENERAL TERMS MAY BE DEFINABLE
IN MORE THAN ONE SPECIFIC WAY.
- ① THE USER HAS TO DECIDE HOW TO TREAT INDIVIDUAL REACTIONS:
 - ① EQUILIBRIUM (DEFAULT)
 - ① SIMPLE DISEQUILIBRIUM
 - ① KINETICS
- ① THE USER MUST ALWAYS BE CONCERNED ABOUT THE ADEQUACY
OF THE SUPPORTING DATA FOR THE PROBLEM AT HAND.

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WORK FOR NNWSI - FY85



- COMPLETED ADDITION OF PRECIPITATION KINETICS CAPABILITY TO THE EQ6 CODE (REPORT BY DELANY, PUIGDOMENECH, AND WOLERY, 1985). REPORT INCLUDES REVIEW OF RATE LAWS FOR PRECIPITATION AND DISSOLUTION.

- WROTE PAPER ON TRANSITION STATE THEORIES AND THEIR APPLICATION IN GEOCHEMISTRY (SPIN-OFF OF THE ABOVE; NEARLY DONE, WOLERY, 1985). THIS PAPER FIXES A BUG IN THE CONVENTIONAL THEORY AND DOCUMENTS IMPORTANT CAVEATS IN THE USAGE OF THE THEORY.

From Delany et al. (1985)

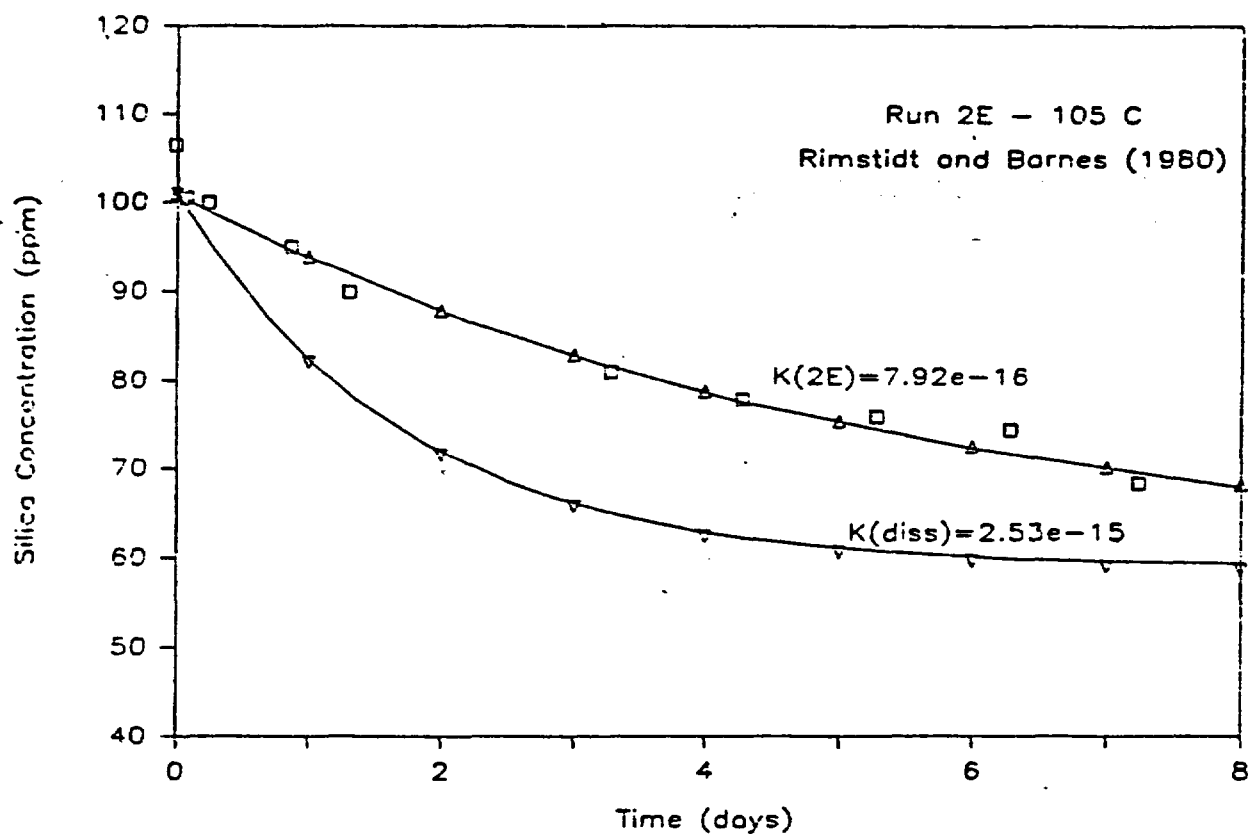


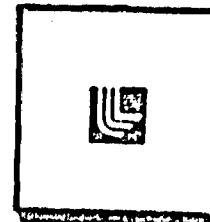
Figure 1. Precipitation growth kinetics of quartz in run 2E of Rimstidt (1979) and Rimstidt and Barnes (1980), shown as the decrease in silica concentration in solution as a function of time. Upper curve: Rimstidt-Barnes TST model with $k_+ = 7.92 \times 10^{-16}$ mol/cm²-sec (see text). Lower curve: same model with $k_+ = 2.53 \times 10^{-15}$ mol/cm²-sec (equation 6-1). Squares: Rimstidt and Barnes experimental data. Triangles: points calculated for closed form solution (see Appendix C).

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WORK FOR NNWSI - FY85 (CONT.)



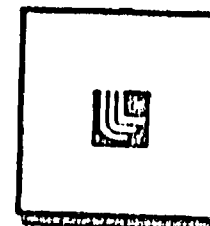
- ① ARE NOW MOVING EQ3/6 AND THE DEVELOPMENT EFFORT ONTO NEW HARDWARE (THE RIDGE COMPUTER). REMAINING FORTRAN 66 CODE MUST BE CONVERTED TO FORTRAN 77. OUR WORK COULD NOT HAVE CONTINUED ON THE CENTRAL LLNL SYSTEM.
- ① HAVE WRITTEN TWO DATA FILE MANAGEMENT CODES (ONE FOR MDA, THE OTHER FOR DATA0), BOTH OF WHICH ARE NOW IN GENERAL USE.
- ① WRITE MCRT USER'S GUIDE. THIS HAS FALLEN BEHIND DUE TO THE CHANGE IN HARDWARE NOTED ABOVE. STILL PLAN TO FINISH THIS BY END OF FY85.

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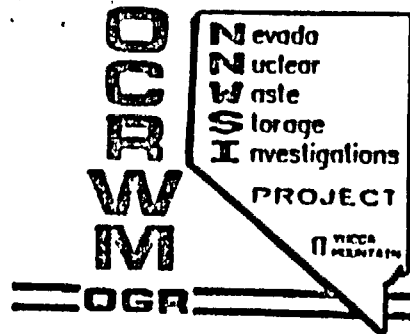
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WORK FOR NNWSI - FY85 (CONT.)



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- ① WRITE STATUS REPORT ON THE THERMODYNAMIC DATA BASE (END OF FY85). WORK IS IN PROGRESS TO GET THE DATA BASE READY FOR THIS REPORT, MOST OF WHICH WILL CONSIST OF LISTINGS OF THE MDA AND DATA0 FILES.
 - ② BEGIN THE ADDITION OF A SORPTION CAPABILITY TO EQ3/6 (INTERIM REPORT DUE END OF FY85). THIS WORK HAS BEEN DELAYED DUE TO THE HARDWARE/FORTRAN 77 CONVERSION.

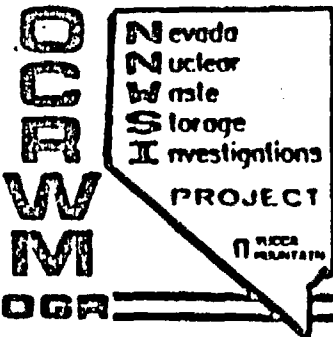


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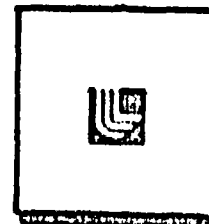


- IMPROVE SOLID SOLUTION MODELING CAPABILITY (INTERIM REPORT ORIGINALLY SCHEDULED FOR END OF FY85, MOVED TO FY86). HAVE WRITTEN NEW CODING TO MAKE EXISTING MOLECULAR-MIXING MODELS WORK ON A ROUTINE BASIS. DELAYED PART CONCERNS ADDITION OF CAPABILITY TO HANDLE SITE MIXING MODELS.

- (2.2.5 MILESTONE) ROGER AINES IS TO WRITE AN INTERIM REPORT ON APPROACHES THAT SHOULD BE TAKEN TO DEVELOP A GLASS/WATER INTERACTIONS MODEL FOR EQ6.



WORK FOR ONWI - FY85



- 0 WROTE PAPER ON PITZER'S EQUATIONS CAPABILITY IN EQ3/6 FOR MRS VOLUME. THESE EQUATIONS ALLOW CALCULATION OF ACTIVITY COEFFICIENTS IN BRINES, BUT THEIR USE IS PRESENTLY RESTRICTED IN SCOPE.
- 0 ASSISTED IN REPOSE TO THE SRP EA'S.
- 0 WROTE REPORT ON INFORMATION NEEDS FOR GEOCHEMICAL MODELING OF BRINE SYSTEMS (LARGELY SLANTED TOWARD SITE CHARACTERIZATION).

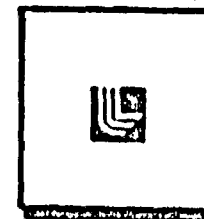
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WORK FOR ONWI - FY85 (CONT.)



-
- ARE DEVELOPING AN EXPERIMENTAL METHODOLOGY FOR DEALING WITH PH IN BRINES.
 - ARE DEVELOPING A NEW SET OF EQUATIONS FOR PREDICTING ACTIVITY COEFFICIENTS IN BRINES, BASED ON MODIFIED DEBYE-HÜCKEL THEORY AND HYDRATION THEORY. THIS IS AMONG OUR MOST SCIENTIFICALLY INTERESTING TASKS.
 - ARE NOW WRITING QA PROCEDURES FOR EQ3/6 WORK. THE SAME PROCEDURES WILL SATISFY THE DRAFT NNWSI REQUIREMENT FOR SOFTWARE QA.

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ESSENTIAL FUTURE WORK FOR NNWSI - FY86 ON



- CONTINUE NECESSARY MAINTENANCE AND DOCUMENTATION OF THE CODES AND DATA BASES. THIS IS ABSOLUTELY NECESSARY FOR QUALITY ASSURANCE PURPOSES AND CRITICAL FOR ACCEPTANCE BY THE OUTSIDE GEOCHEMICAL COMMUNITY.
- COMPLETE ADDITION OF SITE-MIXING MODELS FOR SOLID SOLUTION (IMPORTANT ESPECIALLY FOR CLAYS AND ZEOLITES). AS NEEDED, TAKE SPECIFIC MODELS FOR IMPORTANT PHASES FROM THE LITERATURE, OR DEVELOP OR MODIFY SUCH MODELS.
- COMPLETE ADDITION OF THE SORPTION CAPABILITY TO A MATURE LEVEL. THIS IS AS MUCH A MODEL DEVELOPMENT PROBLEM AS ONE IN CODE DEVELOPMENT. WE NEED TO DETERMINE AN ADEQUATE STATE OF THE ART. THIS IS A MULTI-YEAR ENDEAVOR.

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LESS CERTAIN FUTURE WORK FOR NNWSI - FY86 ON



- 0 MAKE SPECIFIC IMPROVEMENTS TO EQ3/6 FOR MODELING INTERACTIONS INVOLVING METAL CORROSION AND WASTE GLASS. THE POSSIBLE CHANGES HAVE NOT YET BEEN IDENTIFIED OR SHOWN NECESSARY.
- 0 EXTEND EQ6 PHYSICAL MODEL MODES TO INCLUDE THE PSEUDO-1-DIMENSIONAL LEACHING CELL MODE AND/OR A FULL 1-DIMENSIONAL MODE.
- 0 PERFORM OTHER MODIFICATIONS FOR LINKAGE TO A TRANSPORT CODE.

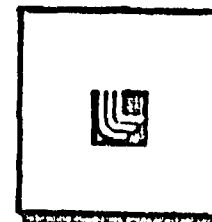
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LESS CERTAIN FUTURE WORK FOR NNWSI - FY86 ON (CONT.)



- ADD PROVISION FOR A GAS PHASE IN EQ6. CURRENTLY, ALL WE CAN DO IS FIX THE FUGACITIES OF SPECIFIC GASES (A PARTIALLY OPEN SYSTEM MODE).
- ADD PROVISION TO EQ3/6 FOR CERTAIN KINDS OF ISOTOPIC FRACTIONATION CALCULATIONS. THIS CAPABILITY EXISTS IN AN OUTSIDE BRANCH VERSION AT CAL TECH AND MIT.

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FUTURE WORK FOR ONWI - FY86 ON



-
- 0 COMPLETE ADDITION OF REDOX DISEQUILIBRIUM MODEL TO EQ6. THIS WAS STARTED THREE YEARS AGO BUT NOT FINISHED DUE TO A PRIORITY RESHUFFLING WHEN ONWI TOOK OVER DIRECT SPONSORSHIP OF EQ3/6 FROM PNL. COMPLETION IS SCHEDULED FOR FY86. THIS HAS BASICALLY THE SAME SIGNIFICANCE TO NNWSI, BWIP, AND OCRD AS IT DOES TO ONWI.
 - 0 WITH THE ABOVE TASK COMPLETED, TIE IT INTO THE KINETIC DRIVER OF EQ6 TO ALLOW MODELING OF REDOX KINETICS. THE SIGNIFICANCE OF THIS CAPABILITY IS ABOUT THE SAME TO ALL THE PROGRAMS.

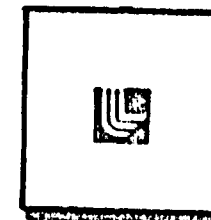
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FUTURE WORK FOR ONWI - FY86 ON (CONT.)



-
- 0 CONTINUED DEVELOPMENT IN FY86 OF OUR NEW EQUATIONS FOR ACTIVITY COEFFICIENTS IN BRINES. THIS HAS SLIGHT SIGNIFICANCE TO NNWSI (BOIL-DOWN SCENARIO). IT MAY BE VERY IMPORTANT TO OCRD SOMEDAY.

 - 0 APPLICATIONS MODELING AND GENERAL ASSISTANCE TO THE SRP.

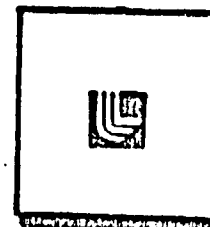
 - 0 NECESSARY MAINTENANCE AND DOCUMENTATION OF THOSE DATA FILES THAT SPECIFICALLY SUPPORT BRINE MODELING CAPABILITIES.

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LESS CERTAIN FUTURE WORK FOR ONWI - FY86 ON



-
- ⑥ ADD THE ACTIVITY COEFFICIENT EQUATIONS OF HELGESON, KIRKHAM, AND FLOWERS (1981), MODIFIED BY OUR ION SIZE AVERAGING TECHNIQUE, TO EQ3/6.

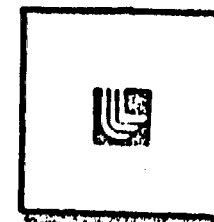
 - ⑥ ADD PRESSURE CORRECTIONS TO THE ACTIVITY COEFFICIENT MODELS.

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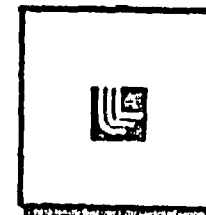
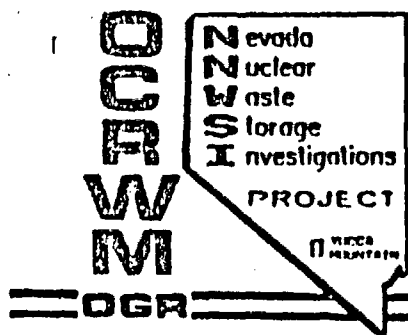
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FUTURE WORK FOR BWIP - FY86 ON



-
- ADD THERMODYNAMIC PRESSURE CORRECTIONS TO EQ3/6. THE DATA CURRENTLY FOLLOW 1 ATM TO 100°C, AND STEAM PRESSURE UP TO 300°C. THE SIGNIFICANCE TO NNWSI IS LOW. SUCH CORRECTIONS MAY TURN OUT TO BE HELPFUL OR NECESSARY FOR SRP AND OCRD.
 - GENERAL ASSISTANCE AND CONSULTING SERVICES.



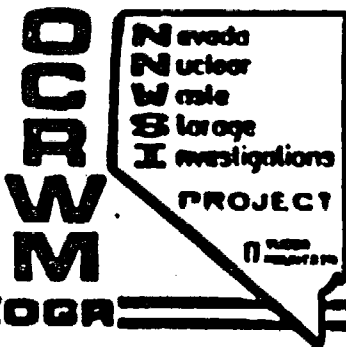
OTHER POSSIBLE FUTURE TASKS

- INCREASE THE TEMPERATURE RANGE OF THE DATA BASE FROM 0-300°C TO 0-500°C (PRESSURE FROM THE UNIVERSITY COMMUNITY. THIS WOULD MANDATE PRESSURE CORRECTIONS.
- ADD A RADIOLYSIS CAPABILITY TO EQ6. HOPEFULLY, MODELING OF INTERACTIONS INVOLVING CHEMICAL SUBSTITUTES (E.G., HYDROGEN PEROXIDE, OXALIC ACID) WILL SUFFICE TO MEET WASTE PROGRAM NEEDS.

ATTENDEES AT NNWSI SEISMIC-TECTONIC WORKING GROUP MEETING JULY 22-23, 1985

(* - attended second day)

Jerry S. Szymanski *	DOE/NV	FTS 575-1503
Michael Voegelé *	SAIC/NNWSI	FTS 575-1460
Chris Pflum	SAIC/NNWSI	FTS 575-1464
Joy Fiore	SAIC/NNWSI	FTS 575-0846
Bruce Crowe	Los Alamos	FTS 843-4299
Al Rogers	USGS	FTS 236-1585
George Brogan	Applied Geosciences Inc.	(714) 838-8545
Howdy Pratt	SAIC/LaJolla	(619) 458-2732
Uel S. Clanton *	DOE/NV	FTS 575-1589
Michael D. Carr	USGS	FTS 467-2504
Bob Raup *	USGS	FTS 776-1273
Fred Donath *	Earth Technology Corp.	(213) 595-6611
James Neal *	SNL	(505 or FTS) 846-0082
Norman Owen *	URS/John A. Blume	(415) 397-2525
Kenneth F. Fox Jr.	USGS	FTS 776-1282
Robert B. Smith	Univ. of Utah	(801) 581-7169
Robert E. Wallace	USGS/Menlo Park	(415) 823-8111
Bob Scott	USGS/Denver	FTS 776-1230
Jack Healy	USGS/Menlo	415-323-8111
John Sass	USGS/Flagstaff	FTS 765-7226 or 602-527-7226
Paul Prestholt *	NRC/Las Vegas	598-6125
Brad Myers *	USGS/Denver	776-1274
Ralph Peters *	SNL/PA	884-4001
Maxwell Blanchard	DOE/NV	FTS 575-1091
Charles Fricker	SAIC/McLean, VA	703-825-4684
Tim Barbour *	SAIC/Golden, CO	303-231-9094
Fred R. Conwell *	SAIC/San Leandro	415-351-7807
Bill Ellis	USGS/Denver	FTS 776-1600
David M. Perkins	USGS/Denver	FTS 776-1616
Frank McKeown	USGS/Denver	776-1575
Joe Litehiser	Bechtel	415-768-7145
Don Emerson *	LLNL	2-6504
Ching Wu *	Bechtel	(415) 882-3728
Neil Norman *	Bechtel	415 768-4035
Leslie J. Jardine *	Bechtel	415 768-4286
John Bredohoeft	USGS	415-322-8111 x2274



Development and Application of EQ3/6

General Applications



(1) ONWI Code Development and Applications

(2) Examples of EQ3/6 Applications

- Hydrothermal Ore Deposits
- Migration of Ruthenium
- Seawater-Rock Interactions
- Sediment-Hosted Ore Deposits

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ONWI Code Development and Applications



- Geochemical Modeling for ONWI Requires the Capability to Deal with Reactions Involving Concentrated Solutions
- EQ3/6 Formerly Limited to Dilute Solutions (Less Than About 1 Molal)
- New EQ3/6 Versions Can Be Used for Brine-Salt Mineral Reactions

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ACTIVITY COEFFICIENTS



The Activity Coefficient of an Aqueous
Species Relates Its Concentration on
the Molal Scale to Its Activity

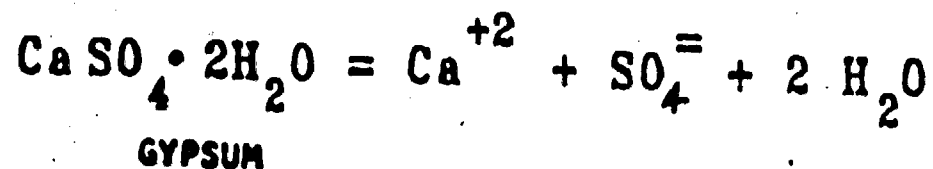
$$a = \gamma m$$

Activities or Thermodynamic Concentrations
Appear in:

- Mass Action Equations
- Kinetic Rate Law Equations

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NRCActivities Appear in Solubility
Calculations

EXAMPLE:



- AT EQUILIBRIUM,

$$K_{\text{GYPSUM}} = (a_{\text{Ca}^{2+}}) (a_{\text{SO}_4^{2-}}) (a_{\text{H}_2\text{O}})^2$$

- THE DEGREE OF DISEQUILIBRIUM IS MEASURED BY THE SATURATION INDEX,

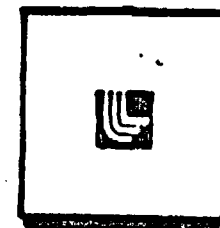
$$SI_{\text{GYPSUM}} = \text{LOG} [(a_{\text{Ca}^{2+}}) (a_{\text{SO}_4^{2-}}) (a_{\text{H}_2\text{O}})^2 / K_{\text{GYPSUM}}]$$

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Geochemical Processes Involving Brines:

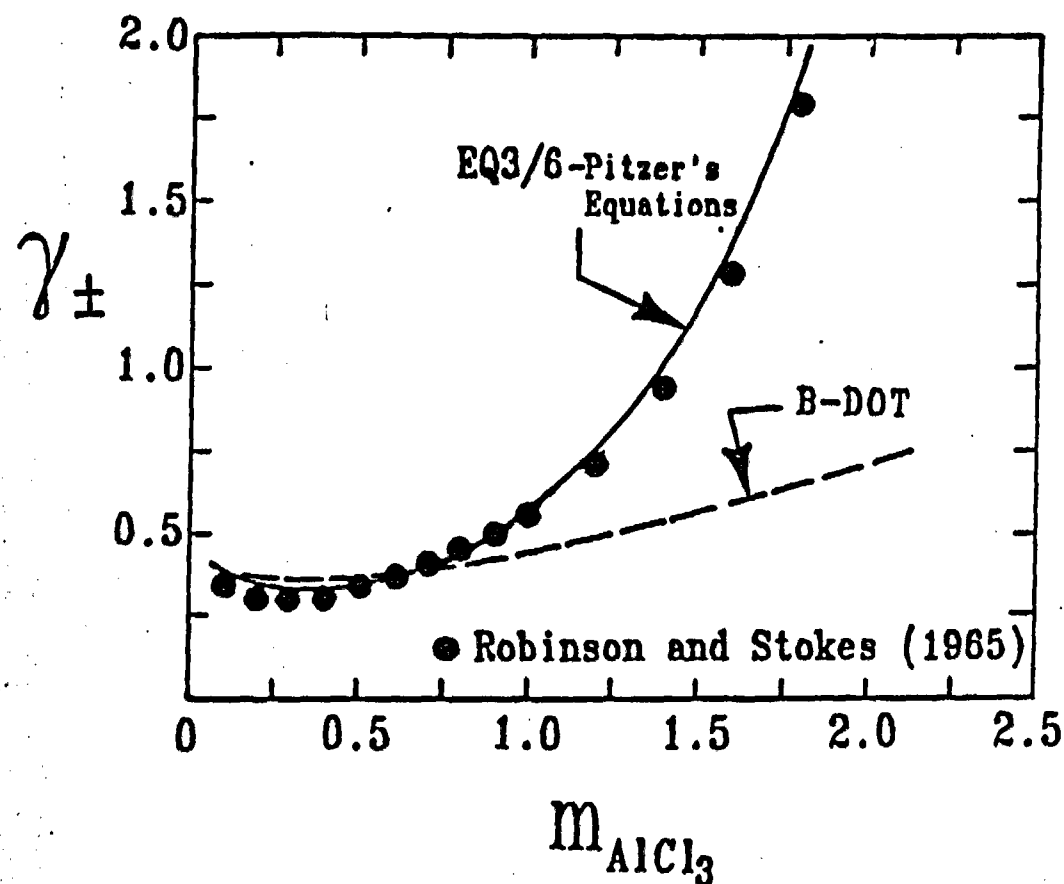
- Formation of Hydrothermal Ore Deposits
- Diagenetic Processes (Oil Field Brines)
- Utilization of Hydrothermal Energy
- Nuclear Waste Disposal

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Pitzer's Equations

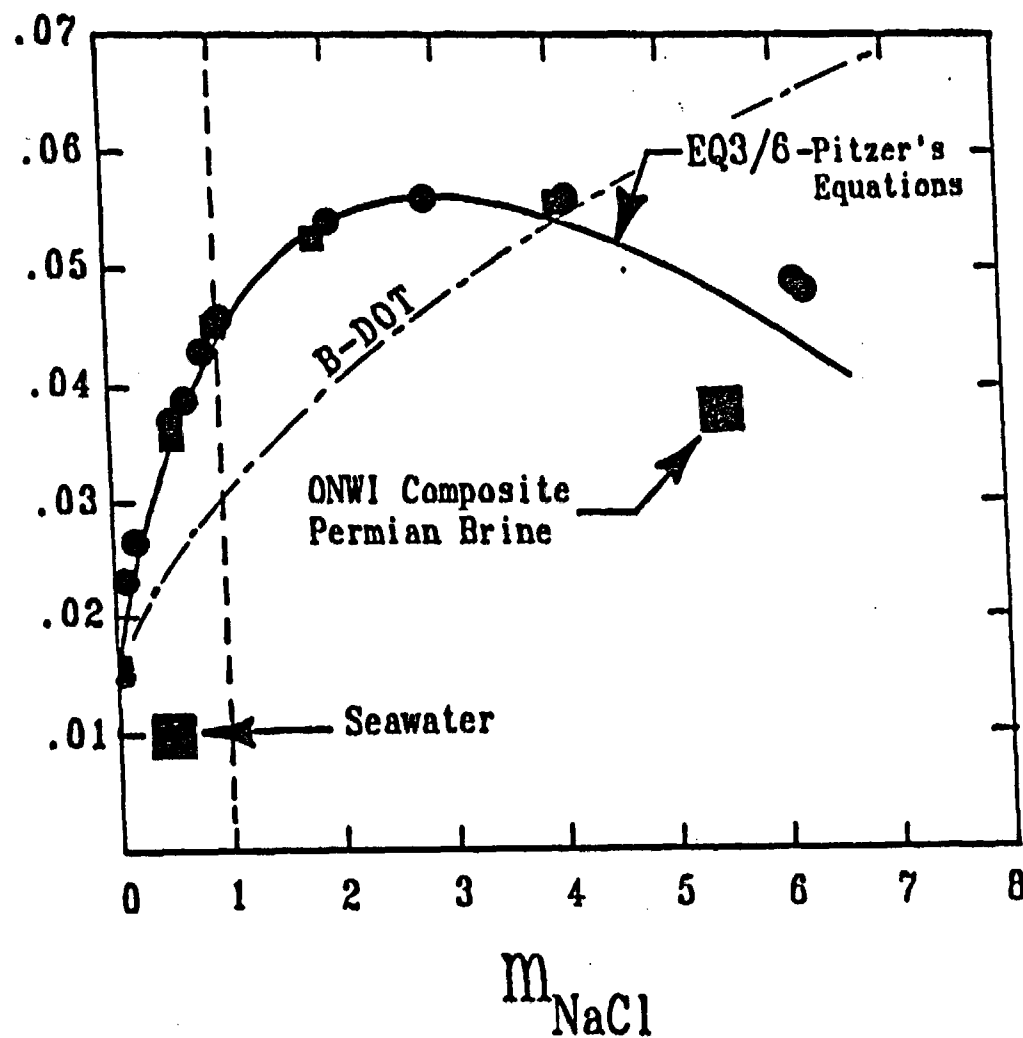


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Pitzer's Equations

 $m_{t,Ca}$ 

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HQS-100-100

Previously Available Activity

Coefficient Options Are Inadequate



- B-DOT and Davies Equations are limited to dilute solutions
- Pitzer's Equations--
 - Requisite data not available for many geologically important components
 - High temperature data rare
 - Can not be extrapolated reliably

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Hydration Theory



- An attempt to use updated versions of some old ideas about activity coefficients
- Basic Idea -- Ions in solution exist primarily as hydrated species
- Likely to handle actinides more readily than Pitzer's equations
- Will Require Less Additional Experimental Effort Than Pitzer's Equations for 'New Species'

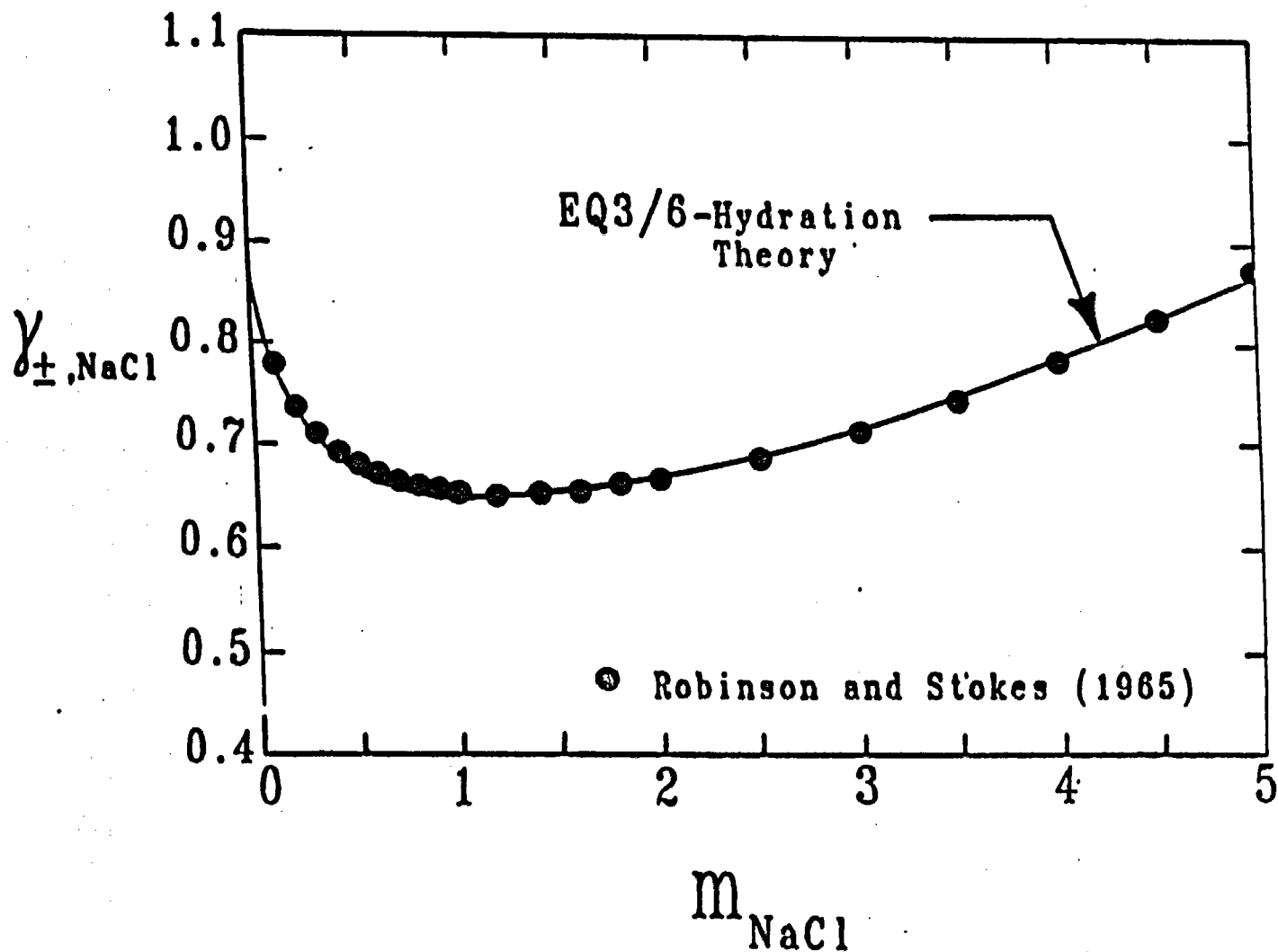
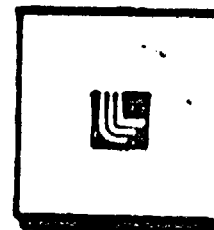
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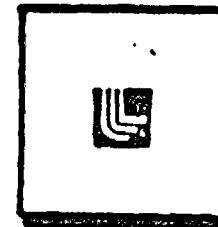
Hydration Theory



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NUCLEAR WASTE
MANAGEMENT**



GARVEN (1982) STUDIED THE FORMATION OF STRATABOUND ORE BODIES (LEAD-ZINC DEPOSITS HOSTED IN CARBONATE STRATA) BY MAKING "GENERIC" SIMULATIONS OF THEIR GENESIS

- **HYDROLOGIC SIMULATIONS OF FLUID FLOW, HEAT TRANSPORT, AND DISPERSION IN TWO-DIMENSIONAL SEDIMENTARY BASINS USING A FINITE ELEMENT CODE**
- **EQ3/6 SIMULATIONS OF THE PROCESS OF LEAD AND ZINC SULFIDE DEPOSITION AT THE ORE-FORMING SITE**
- **THE TIME REQUIRED FOR A SINGLE REACTION-PATH CALCULATION WAS ABOUT THE SAME AS THAT REQUIRED FOR A HYDROLOGIC CALCULATION CORRESPONDING TO THE ENTIRE TIME INTERVAL UNDER STUDY- HENCE, THE CALCULATIONS FOR METAL TRANSPORT ACROSS THE BASIN AND THE GEOCHEMICAL INTERACTIONS WERE NECESSARILY DECOUPLED.**

GEOCHEMICAL MODELS FOR STRATABOUND ORE GENESIS (AFTER GARVEN, 1982, IN TURN AFTER OTHERS)

TRANSPORT MODEL

**I. METALS TRANSPORTED IN
LOW-SULFUR FLUID**

**II. METALS TRANSPORTED IN
SULFATE-BEARING FLUID**

**III. METALS AND SULFIDE
TRANSPORTED TOGETHER IN
THE SAME FLUID**

REASONS FOR DEPOSITION

A) MIXING WITH H_2S -BEARING FLUIDS

B) REACTION WITH IRON SULFIDES

C) THERMAL DEGRADATION OF ORGANICS

SULFATE REDUCTION BY

→ ***A) BACTERIAL DESTRUCTION OF ORGANICS**
B) NON-BACTERIAL DESTRUCTION OF ORGANICS

***C) REACTION WITH METHANE**

D) ENCOUNTERING PETROLEUM

***E) REACTION WITH IRON SULFIDES**

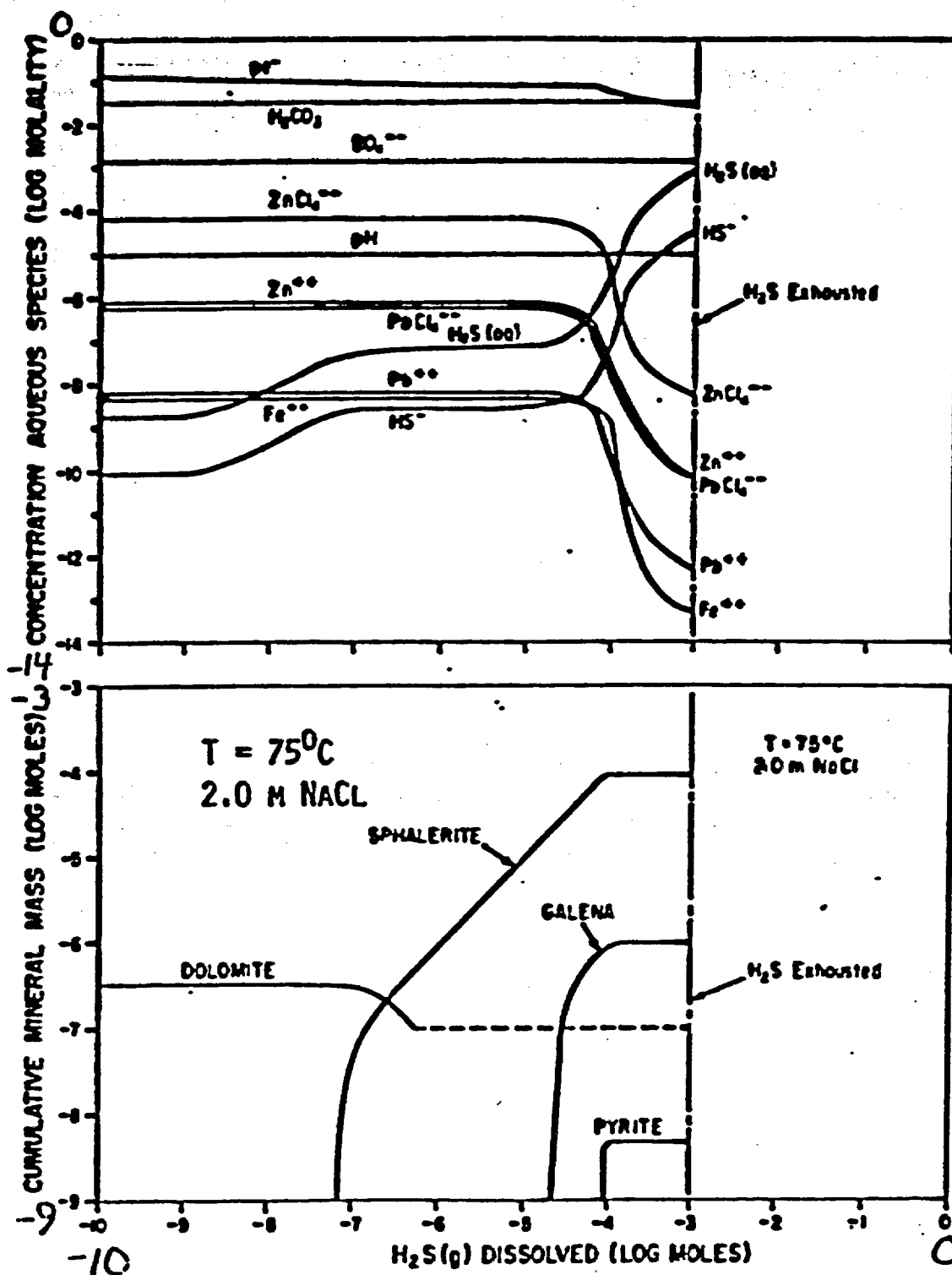
***A) REACTION WITH THE HOST ROCK AND RISE
IN PH**

→ ***B) TEMPERATURE DROP**

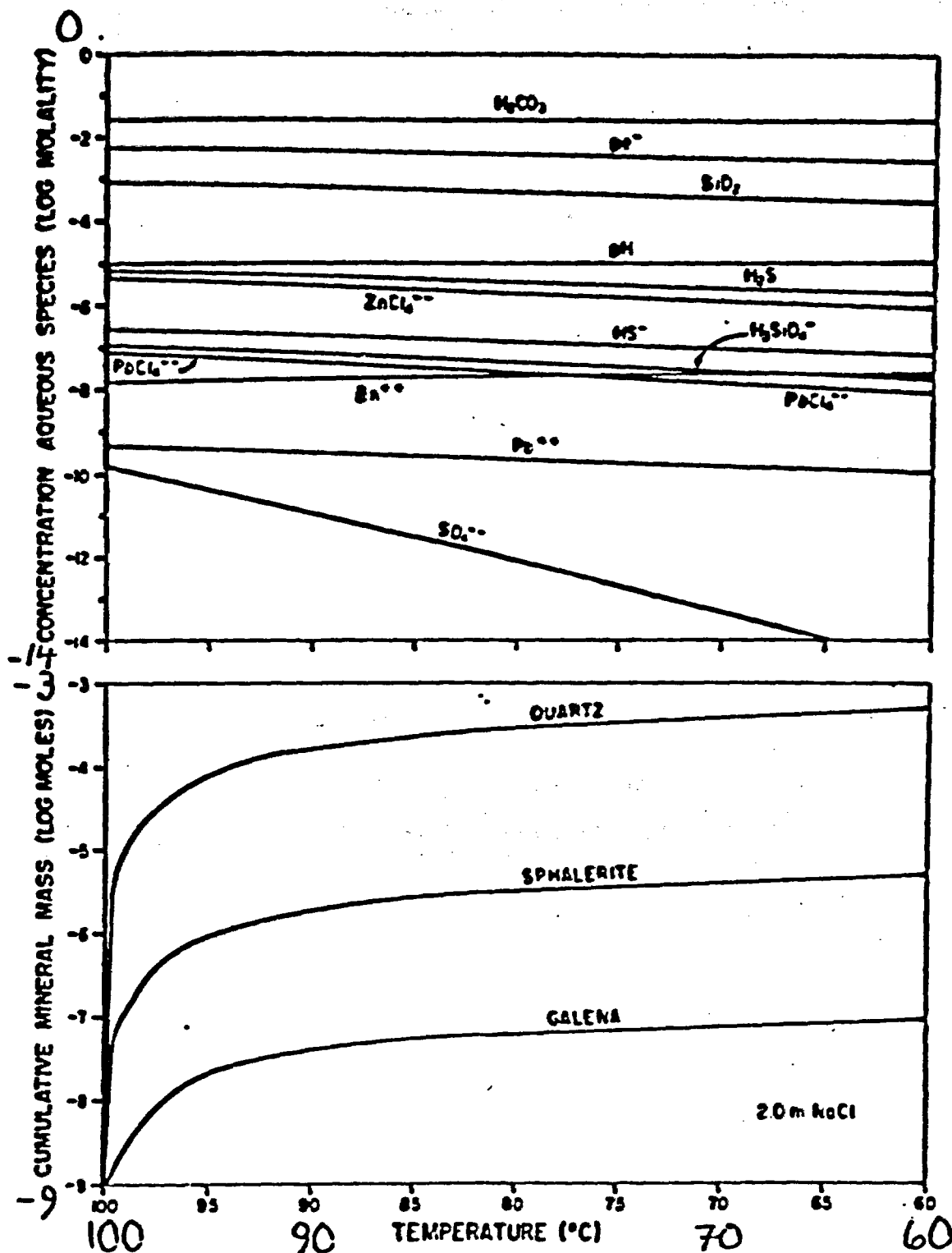
**C) DECREASED STABILITY OF CHLORIDE COMPLEXES
DUE TO FLUID MIXING**

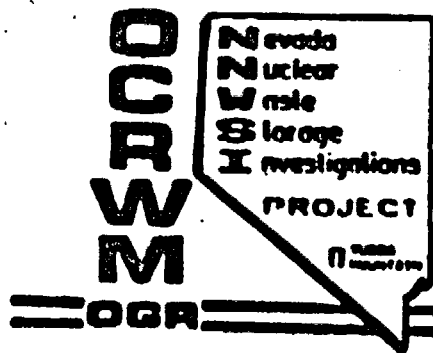
***FEASIBILITY SHOWN BY GARVEN (1982) BY THE USE OF EQ3/6 SIMULATIONS**

GARVEN (1982): EQ3/6 SIMULATION OF REACTION OF A METAL-SULFATE
BRINE WITH H_2S PRODUCED BY BACTERIAL DEGRADATION OF ORGANIC
MATTER- TEST OF MODEL II-A

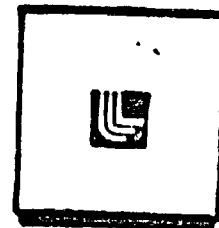


GARVEN (1982): EQ3/6 SIMULATION OF PRECIPITATION OF LEAD AND ZINC SULFIDE IN RESPONSE TO COOLING A METAL-SULFIDE BRINE FROM 100°C TO 60°C- TEST OF MODEL III-B

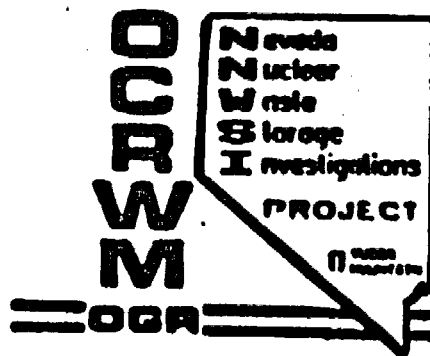




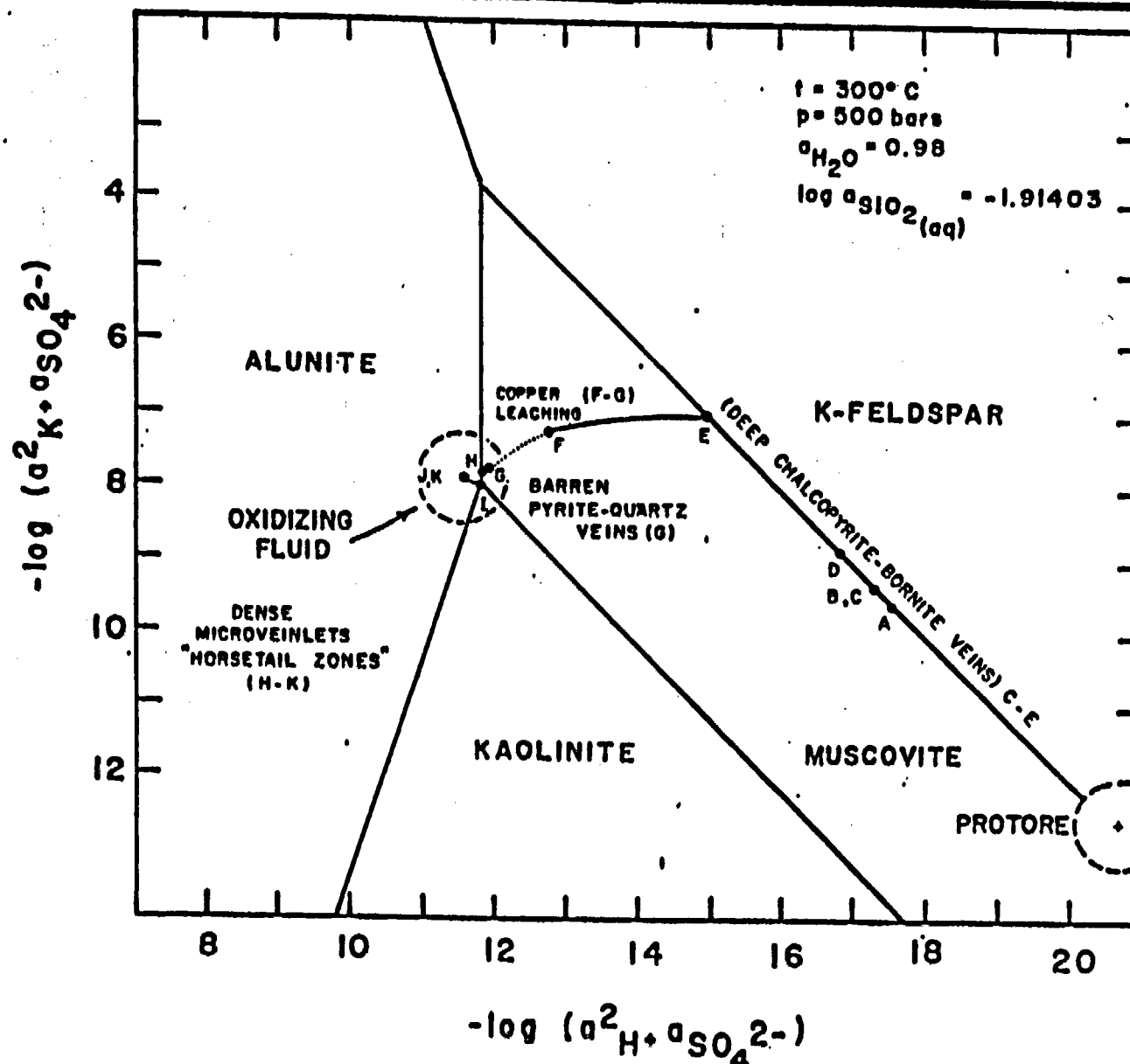
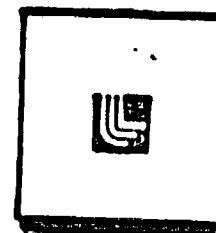
Porphyry Copper Deposits



- o Brimhall (1980) Used EQ3/6 to Confirm His Field-Based Hypothesis on the Ore-Forming Processes in the Butte Porphyry Deposit
- o EQ3/6 Calculations Reproduced the Mineral Assemblages Observed at Butte at Different Stages in the Ore-Forming Process
- o Serves as a Verification of a Field-Based Model Using EQ3/6 Modeling



Porphyry Copper Deposits



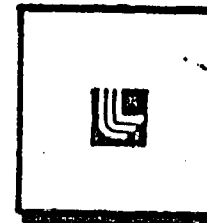
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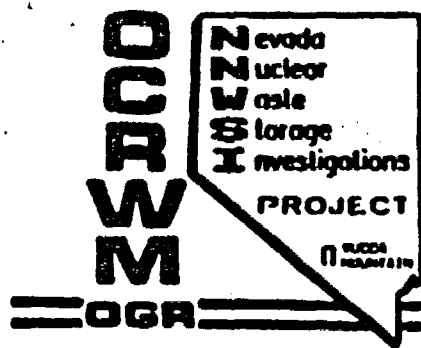
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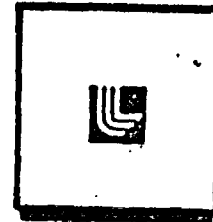
COLES AND RAMSPOTT (1982) FOUND THAT RUTHENIUM MIGRATED
IN GROUNDWATER FROM A NUCLEAR EXPLOSION CAVITY AT NTS.



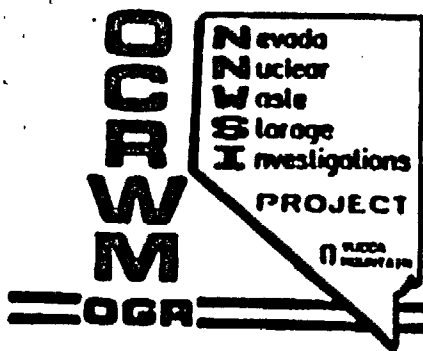
- LABORATORY K_D MEASUREMENTS IMPLIED THAT SUCH MIGRATION WOULD NOT OCCUR.
- YET RU APPEARED AT A SATELLITE WELL AS THE SAME TIME AS TRITIUM.
- RU HAS A COMPLICATED SOLUTION CHEMISTRY, AS DO THE ACTINIDES.



RUTHENIUM MIGRATION (CONT.)



- NO DEFINITE EXPLANATION WAS FOUND. POSSIBILITIES INCLUDE
- THE RU STOCK SOLUTION IN THE K_D MEASUREMENTS LIKELY CONSISTED MOSTLY OF THE HIGHLY CHARGED CATIONIC COMPLEX $\text{Ru}_4(\text{OH})_{12}^{++++}$, A SMALL POLYMERIC SPECIES AND PROBABLE EXCELLENT SORBER. IT MAY HAVE BEEN KINETICALLY STABLE FOLLOWING DILUTION FOR THE EXPERIMENTS.
- ALTERNATIVELY, IF EQUILIBRIUM WAS OBTAINED, RU MAY HAVE BEEN SORBED OR PRECIPITATED IN THE LABORATORY BUT NOT IN THE FIELD DUE TO DIFFERENCES IN PH AND TOTAL RU CONCENTRATION.

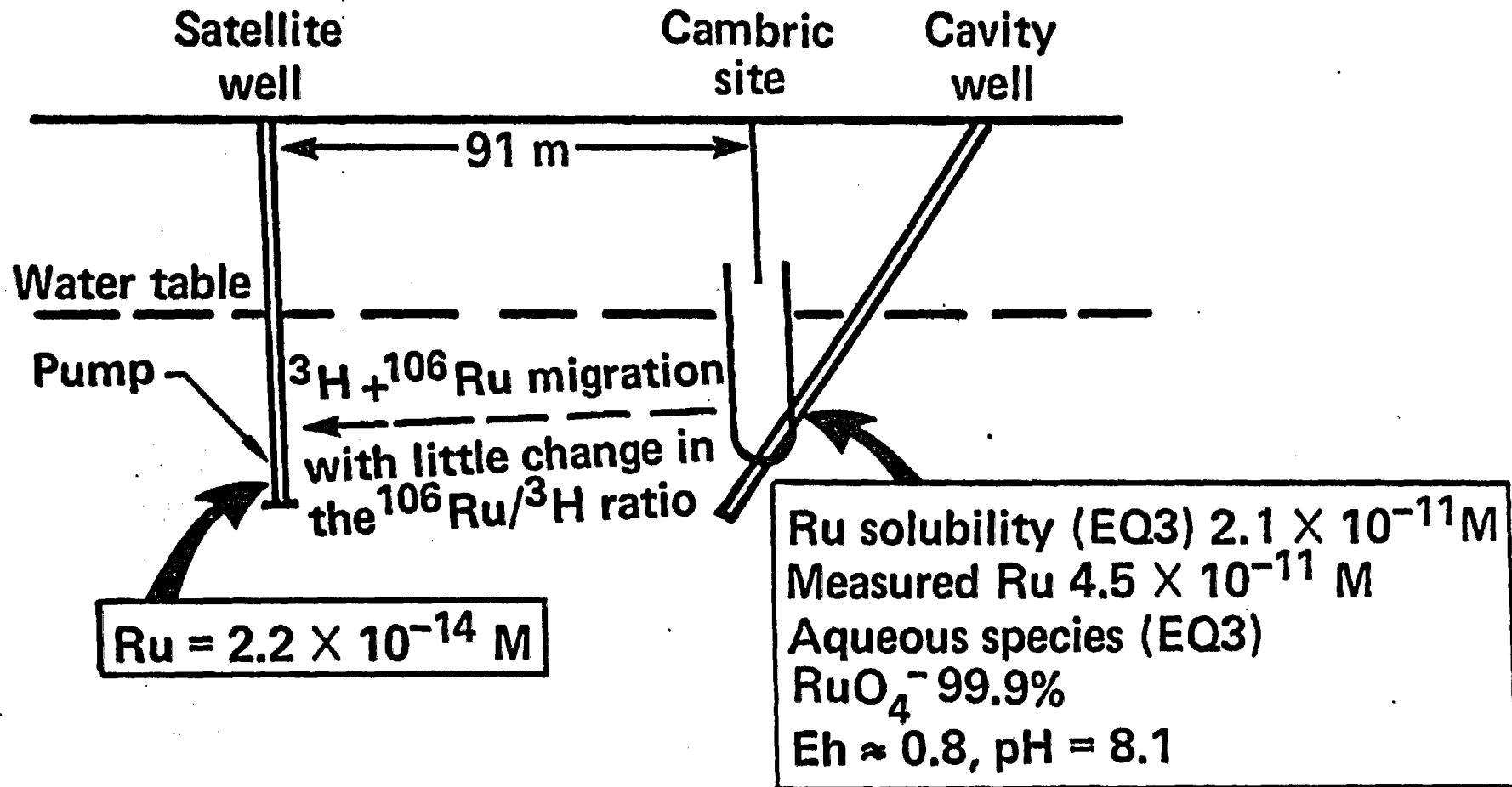


RUTHENIUM MIGRATION (CONT.)



- RARD (1985) REVIEWED THE CHEMISTRY AND THERMODYNAMICS OF RU SPECIES. ISHERWOOD (1985) USED HIS DATA IN EQ3/6 TO TRY TO UNRAVEL THE CAMBRIC PUZZLE.
- EQ3NR CAME VERY CLOSE TO PREDICTING THE CONCENTRATION OF RU IN THE CAVITY WATER (NEXT VIEWGRAPH).

Why did Ruthenium migrate at Cambric Site (NTS)?



Do laboratory measurements reflect in situ conditions?

With a K_d measured in the lab of 10^3 ml/g , ruthenium should have migrated $< 10 \text{ cm}$.

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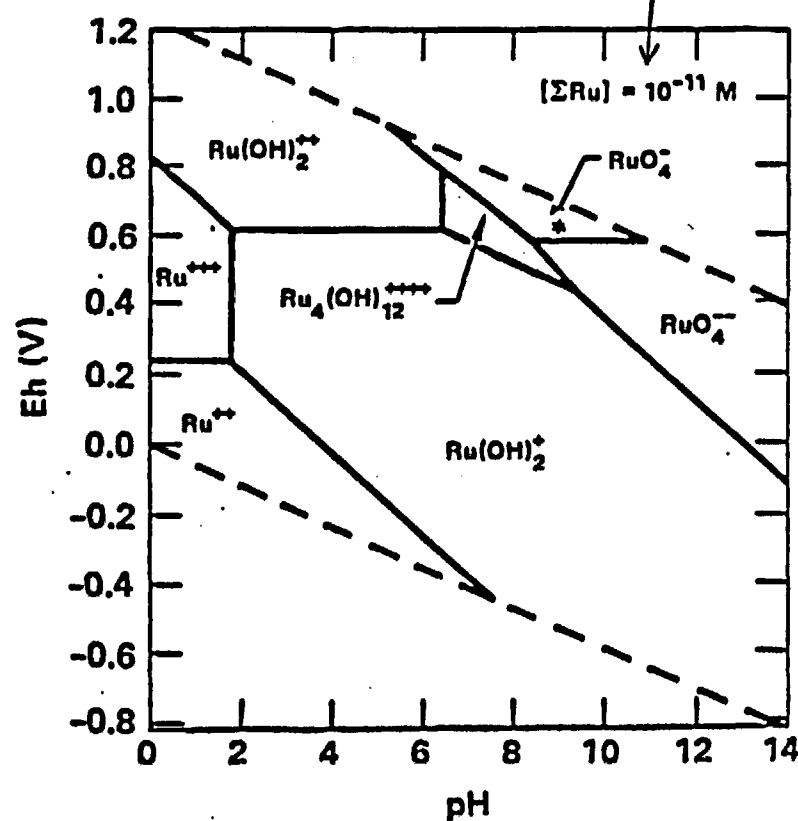
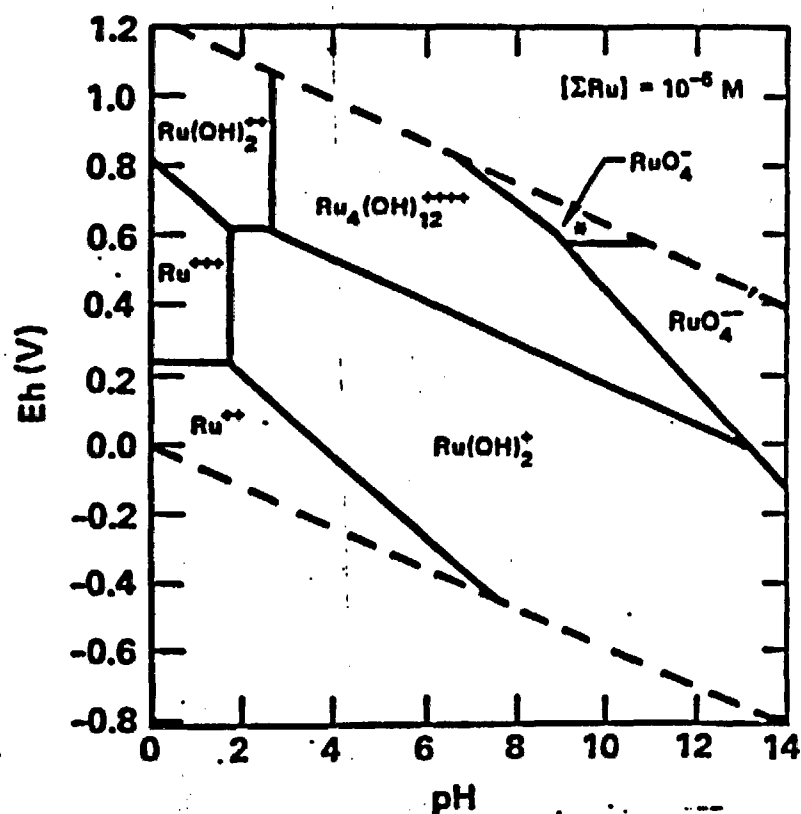
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RU SPECIATION DEPENDS ON PH, EH, AND TOTAL RU
BECAUSE OF THE EXISTENCE OF THE 4:12 COMPLEX



TOTAL RU CLOSEST TO
CAVITY WATER



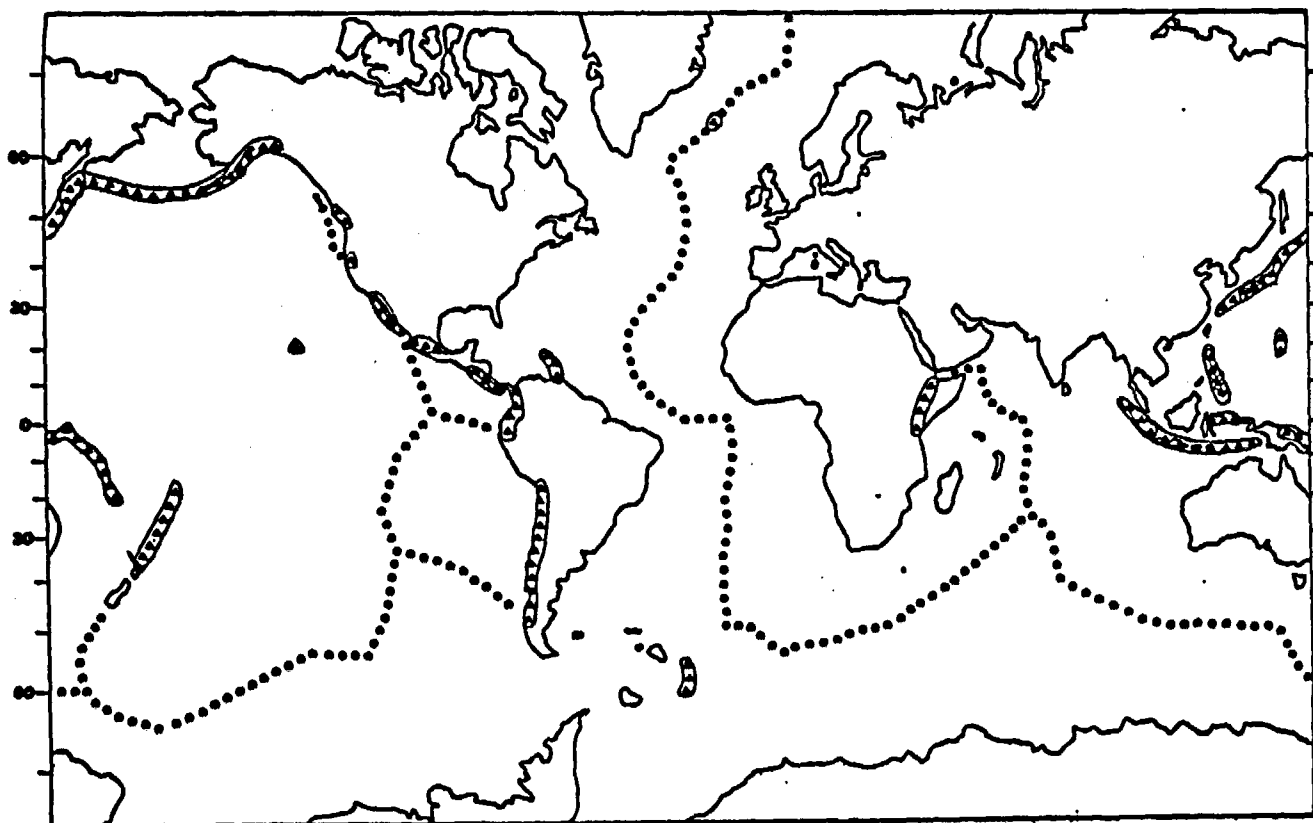
• CAMBRIC WATER

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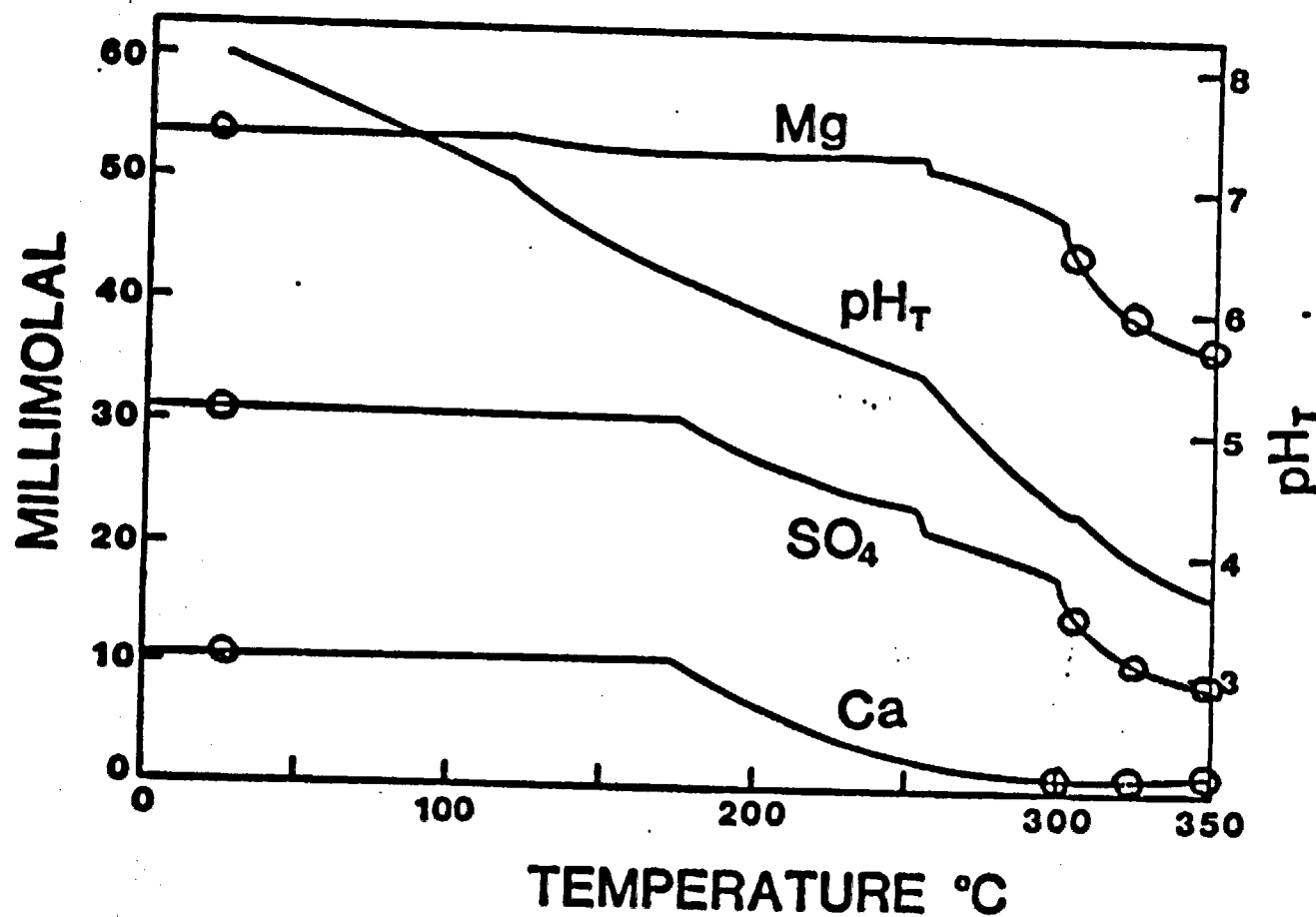
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JANECKY (1982) USED EQ3/6 SIMULATIONS ALONG WITH HIS ORIGINAL EXPERIMENTAL INVESTIGATIONS TO

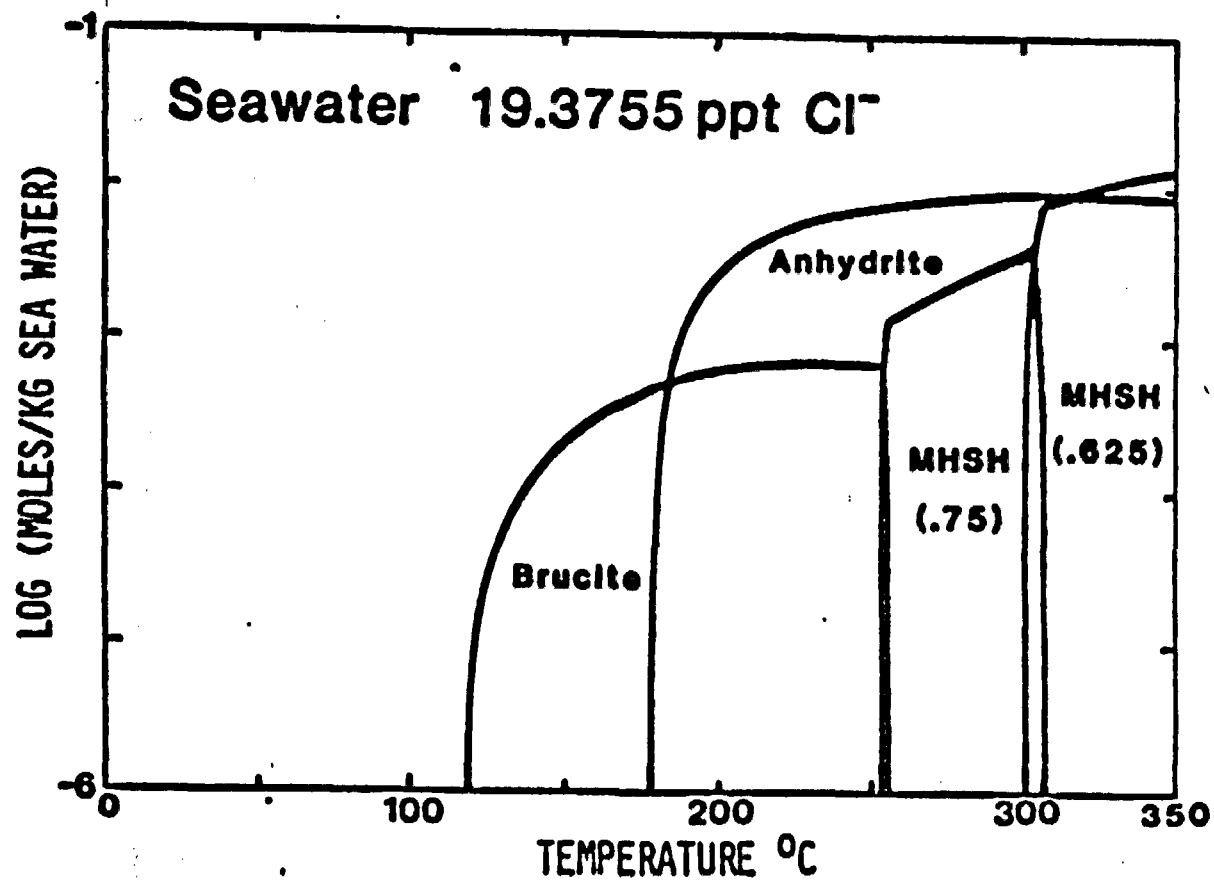
- **DETERMINE THE CONSEQUENCES OF HEATING SEA WATER TO 350°C**
 - **EQ3/6 WAS USED TO HELP DETERMINE THE THERMODYNAMIC PROPERTIES (E.G., SOLUBILITIES) OF THE MAGNESIUM HYDROXYSULFATE HYDRATE (MHS) PHASES**
- **STUDY THE REACTION OF SEA-FLOOR PERIDOTITES (LHERZOLITE AND HARZBURGITE) WITH HYDROTHERMAL SEA WATER TO PRODUCE SERPENTINITES**

JANECKY (1982): EQ3/6 PREDICTIONS OF CHANGES IN THE COMPOSITION OF SEA WATER HEATED TO 350°C AT 500 BARS PRESSURE (CARBONATE MINERALS NOT ALLOWED TO FORM, CONSISTENT WITH EXPERIMENTAL RESULTS)



○ = EXPERIMENTAL DATA POINTS

JANECKY (1982): EQ3/6 PREDICTIONS OF MINERALS PRECIPITATING FROM SEA WATER
HEATED TO 350°C AT 500 BARS PRESSURE (CARBONATE MINERALS NOT ALLOWED TO FORM)



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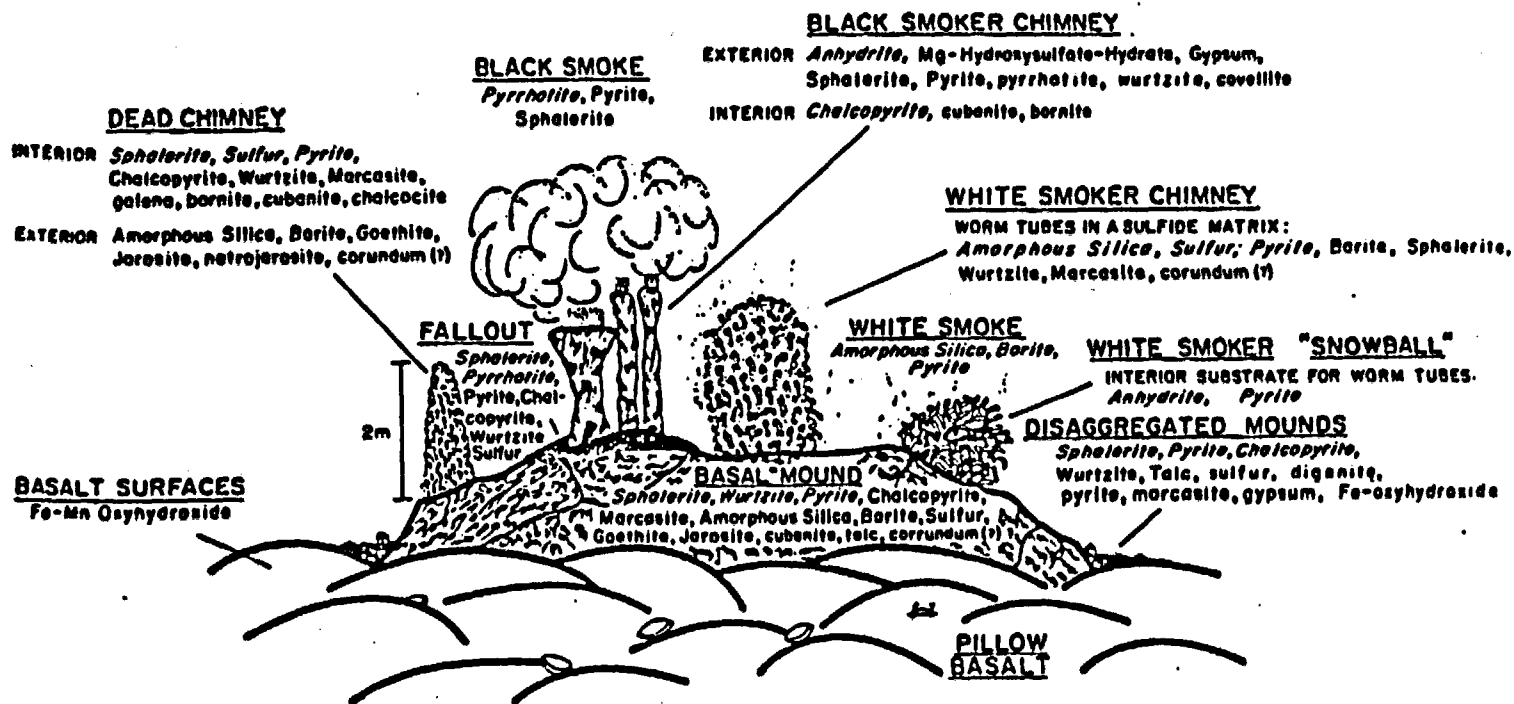
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Black Smoker Hydrothermal Vents



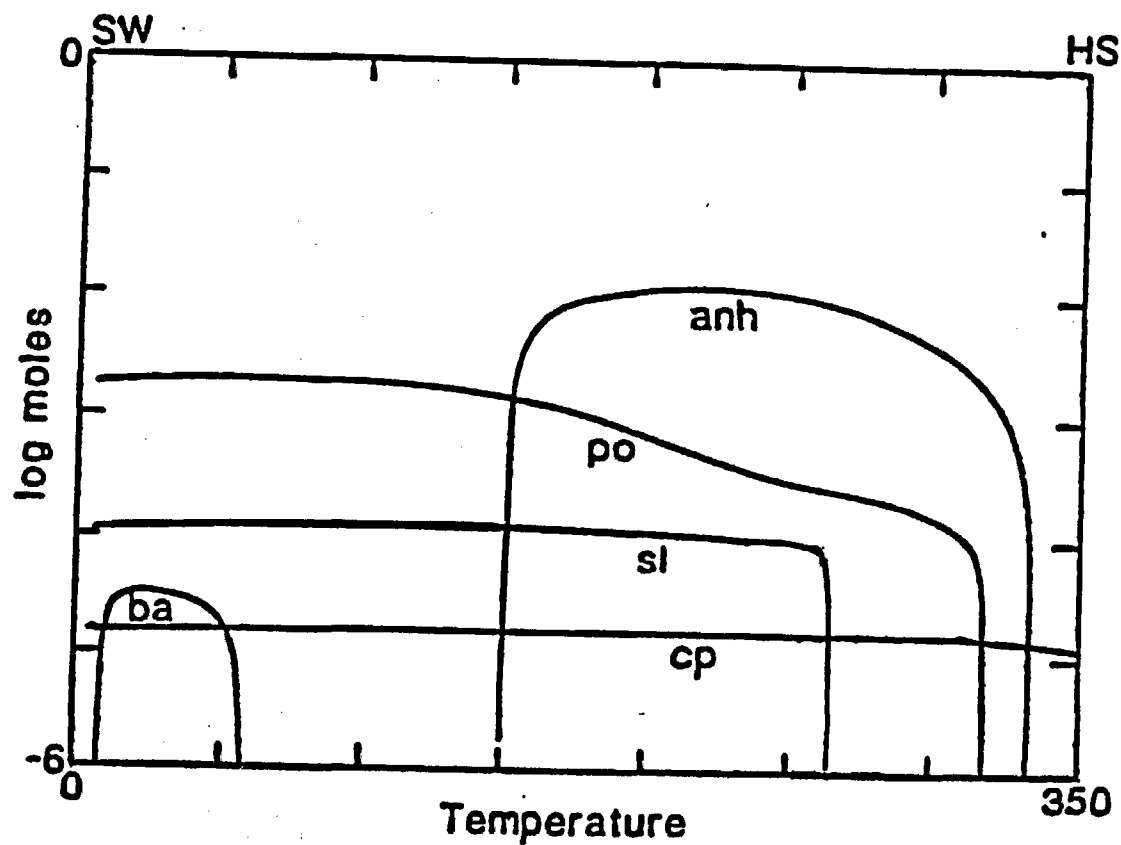
SCHEMATIC DISTRIBUTION OF HYDROTHERMAL VENT MINERALS



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REPORT

Black Smoker Hydrothermal Vents



anh = anhydrite
po = pyrrhotite
sl = sphalerite
cp = chalcopyrite
ba = barite



To: Don Vitt

United States Department of the Interior

GEOLOGICAL SURVEY
RESTON, VA. 22092

OFFICE OF THE DIRECTOR

In Reply Refer To:
WGS-Mail Stop 106

JUN 27 1985

Mr. Bernard C. Rusche
Office of Civilian Radioactive
Waste Management
U.S. Department of Energy
Washington, D.C. 20585

ACTION

CC: VIAH
CC: KUMIL
CC: BC'S
CC: Blaylock

Dear Mr. Rusche:

As you are aware, the U.S. Geological Survey (USGS) has been reviewing its activities in the Department of Energy's (DOE) nuclear waste repository program.

With respect to the salt and basalt programs, we have been meeting with various elements of DOE and have provided review comments concerning relevant DOE documents. Since we do not perceive significant problems with our participation in these programs, we have not reviewed those activities very extensively.

In contrast, our involvement with the Nevada Nuclear Waste Storage Investigations (NNWSI) program is much greater, and concern has been expressed about our activities in NNWSI; therefore, we have concentrated our review in that area.

The USGS has been participating with DOE's Waste Management Project Office (WMPO) in an ever-expanding program since 1977. During this time period, the USGS's role has been in assessing regional geologic, seismologic, and hydrologic factors, and in analyzing the complex issues associated with the unsaturated zone of the tuffs at Yucca Mountain.

As one would expect, these two major roles come naturally to the USGS, being primarily a scientific organization.

Now that the Draft Environmental Assessments have been released for public comment and the process is moving toward site characterization for licensing, the primary focus is shifting to investigations of the rock in which the repository will be constructed.

Much remains to be completed in the geohydrologic investigations of the Yucca Mountain site and environs. Development of a satisfactory understanding of the specific repository conditions and their interaction

RECORD COPY

Mr. Bernard C. Rusche

2

with the host rock must consume an increasingly large portion of the available resources. The USGS is well qualified and prepared to complete the technical investigations necessary for license application. We are also prepared to defend fully our scientific investigations and findings. Furthermore, we are committed to comply with the basic administrative requirements to fulfill the DOE programmatic needs.

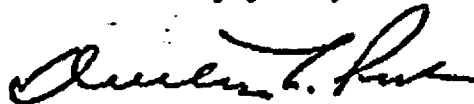
However, the collection and interpretation of specific scientific findings do not in themselves provide the full documentation for licensing review. The facts must be integrated and measured against some legally accepted scale or criteria; the forensic documentation for the licensing process is critical. Preparing such material requires very specific talents, organization, and experience. The USGS is not organized to provide this type of service. Secondly, the USGS has a further obligation to the Government and the public to demonstrate impartiality in its statements. We must retain our position as a disinterested party.

Consequently, we recommend that DOE employ an experienced geologic and engineering organization to perform this major integrating and advocating function. Such an organization should be able to understand both the scientific and the regulatory language and could then translate the technical information from the USGS into the correct terms and format to address the regulations for the DOE.

Our staff is prepared to participate with the NNWSI management of the DOE to identify the specific elements of the program that could remain with the USGS and those that could be assigned to the new organization.

We recognize the very complex task that DOE has in proving an adequate disposal site, and we remain committed to assist you. Should you wish to discuss this further, we would, of course, be willing to do so.

Sincerely yours,

A handwritten signature in dark ink, appearing to read "Dallas L. Peck", written in a cursive style.

Dallas L. Peck
Director

NNWSI Seismic/Tectonic Position Paper

URS/John A. Blume

PROPOSED OUTLINE

July 19, 1985

3.5.2 Seismic Design Parameters

A. Introduction

- 1. Purpose:** propose procedures for developing seismic design parameters
- 2. Topics:**
 - o Classification of facilities**
 - o Design ground motion definitions**
 - o Proposed methodology**
 - o Data needed to refine methodology**

B. Classification of Facilities

- 1. Pre closure**
URS/Blume Classification
- 2. Post closure**
DOE/Weston definition for Waste Isolation

C. Vibratory Ground Motion

- 1. Approaches for other important facilities**
 - a. Two-levels of ground motion for important facilities**
 - b. Deterministic approach for NPPs**
 - c. Probabilistic approach for SEP NPPs**
 - d. Probabilistic approach for DOE facilities**

2. Proposed Definitions for Waste Repository

- a. Pre closure
- b. Post closure

3. Proposed Methodology

- a. Surface
- b. Subsurface

D. Fault Displacement

1. Different Manifestations

- a. Surface rupture
- b. Subsurface rupture at repository depth
- c. Near-fault strain in repository
- d. Relationship among phenomena above

2. Proposed Methodology

E. Data Needed to Support These Methodologies (Preliminary List)

1. Vibration Ground Motion

- a. Regional attenuation functions (surface, subsurface).
- b. Site specific data to adjust regional attenuation functions for site.
- c. Map of ~~capable~~ faults within 100 km (approx.) of site.
possibly seismicogenic

2. Fault Displacement

- a. Locations and rupture histories of faults passing through the repository or within 100 m (approx.) of repository facilities (surface and subsurface).
- b. Friction and average shear stress on faults.

Development and Application of EQ3/6

Waste Package Applications



- EQ3NR

- Electroneutrality Calculations

- Solubility Calculations:

- Uranium

- Americium

- EQ6

- Concentration by Boiling

- Open System 100°C, J-13 Water

- Rock/Water Interaction

- Closed System 150°C, Tpt Tuff + J-13 Water

EQ3NR APPLICATIONS

Electroneutrality



- Purpose:

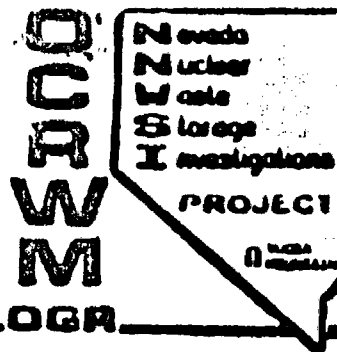
To evaluate the accuracy of all analytical data before it is used in any EQ3/6 applications.

- Principle: Electrolyte solutions are electrically neutral.

$$\sum |z_{cations}| m_{cations} = \sum |z_{anions}| m_{anions}$$

- Error:

±5%, maximum error considered acceptable.



Average J-13 Fluid Analysis[†] LLNL Laboratory Supply



Input file name: j13ave created 09/20/84 creator: j. delany
analysis of j-13 water run as control blanks.
reported by v.m. overby (7/18/84).

average of all data for j-13 analyses:

cations (table 1d)
anions (table 2a)

hco3- average of 13 analyses
(co2 analyzer, reported)

1/14/85)

reference: overby, v.m., 1984, reaction of the topopah spring tuff
with j-13 well water at 120 c: lawrence livermore
national laboratory, ucr1-53574.

```

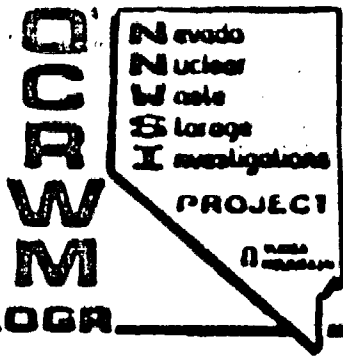
undit.
temp= 25.
rho= 1.0 tdepth= 0. tdepth= 0.
fap= -0.68 uredon=
tblb= 0. toldl= 0. toldl= 0.
itern= 0
iaptl-10= 0 0 0 0 0 0 0 0 0
iapgl-10= 0 0 0 0 0 0 0 0 0
iprnl-10= 0 0 0 0 0 0 0 0 0
ldbgl-10= 0 0 0 0 0 0 0 0 0
uwbale
umod= 0 uaction= nat
hr= -7.6 16
li= .042 3
na= 43.9 3
k= 5.11 3
ca= 12.5 3
mg= 1.92 3
al= .012 3
fe= .006 3
sio2(aq)= 57.76 3
f= 2.2 3
cl= 6.9 3
no3= 9.6 3
hco3= 125.3 3
so4= 18.7 3
undit.

```

pH	7.6
Li	0.042
Na	43.9
K	5.11
Ca	12.5
Mg	1.92
Sc	0.035
Al	0.012
Fe	0.006
Si	27.0
NO ₃	9.6
F	2.2
Cl	6.9
HCO ₃	125.3
SO ₄	18.7

All units in mg/l except pH.

[†]The average analysis is thought to closely represent the
LLNL laboratory supply on any given day.



EQ3NR APPLICATIONS

Saturated Solutions



- Purpose:

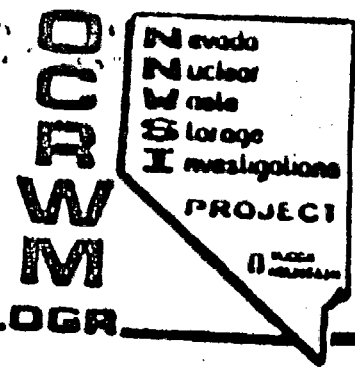
To determine maximum concentrations in solution based on solubility constraints.

- Solubility:

The maximum amount of a substance that can be dissolved in a solution, consistent with thermodynamics

- K_{sp} :

The product of the thermodynamic activities of the ions in solution is a constant.



EQ3NR APPLICATIONS

Saturated Solutions Con't



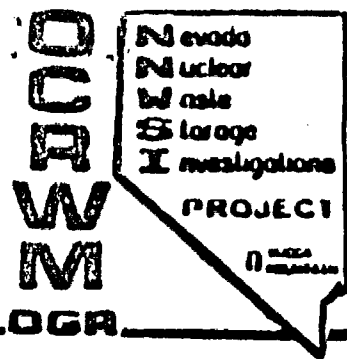
- EQ3NR parameters that can be used to study solubilities:

Temperature

Pressure

Nature of the solid phase

Solution Composition (e.g. pH, ionic strength)

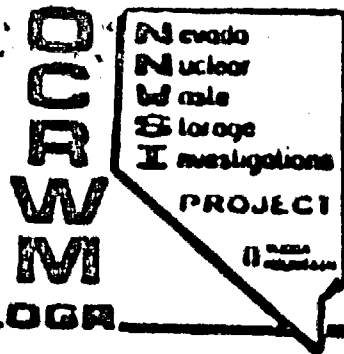


EQ3NR Solubility Studies

NNWSI Project



- Use experimental data that is currently becoming available through the Waste Package Task, to simulate laboratory results.
- Validate thermodynamic data in the data base.
- Simulate measurements being made in J-13 water.
- Make further calculations and predict effects of changing conditions.

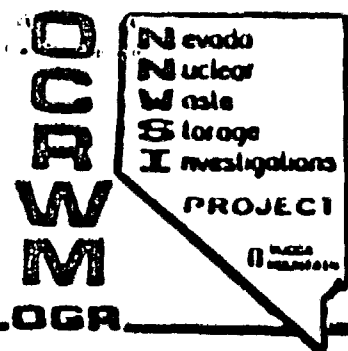


ACTINIDE DATABASE STUDY

(2/85 to Present)



- Uranium 129 species currently under revision
- Americium 34 species currently under revision
- Plutonium 42 species work began 7/15/85
- Technetium 23 species
- Neptunium (planned fall 1985)



EQ3/6 Database Status

July 12, 1985



DATA0S29

38 Elements

505 Aqueous Species

419 Minerals

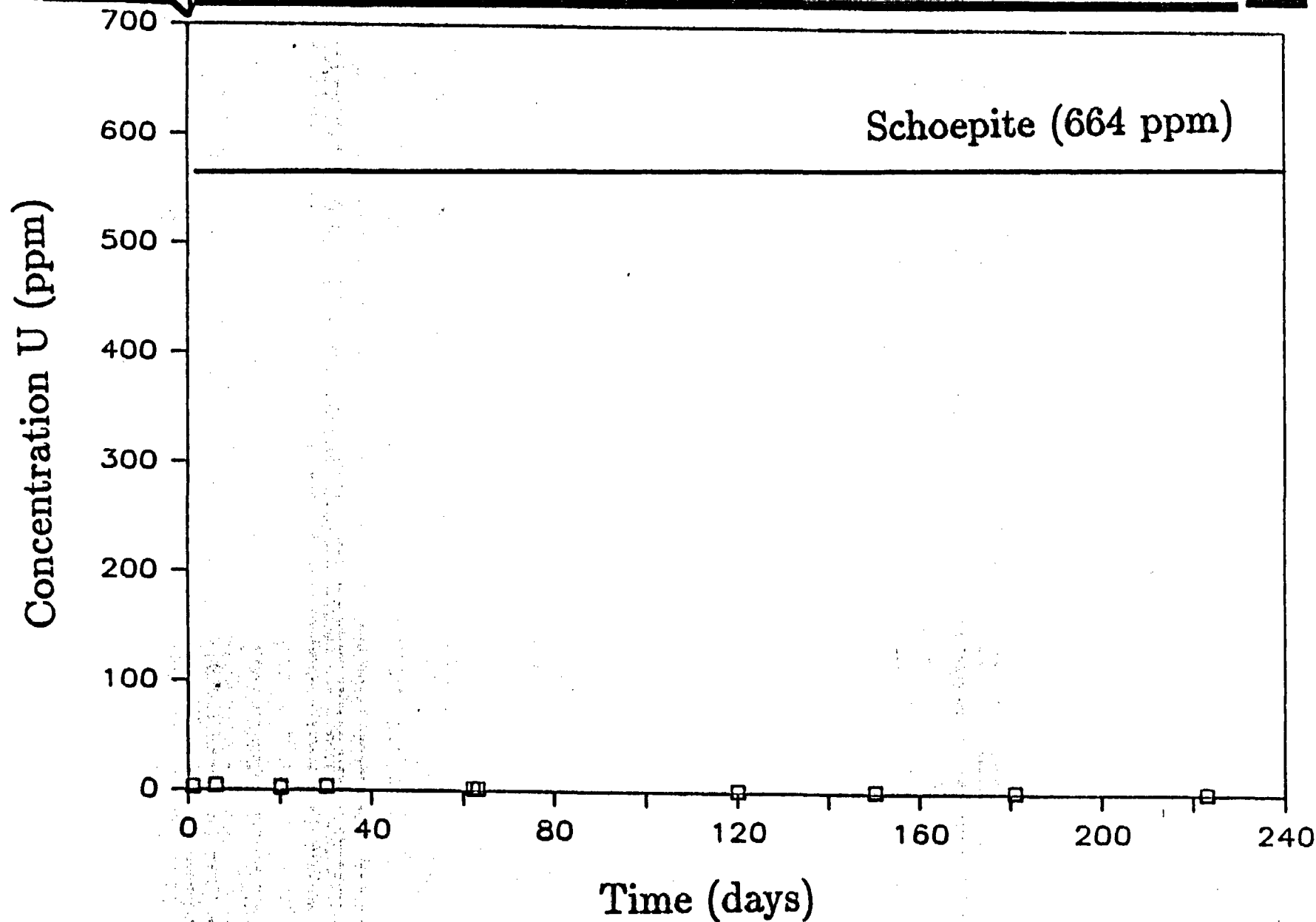
8 Gases

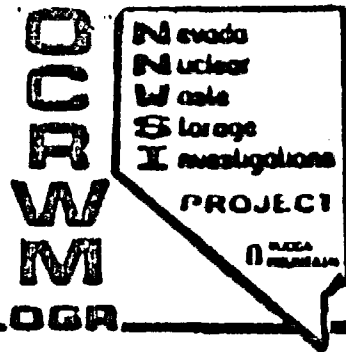
7 Solid Solutions

977 Total Species

EQ3NR Solubility Constraint = Schoepite

J-13 + Uranium (25°C, pH 8.1)





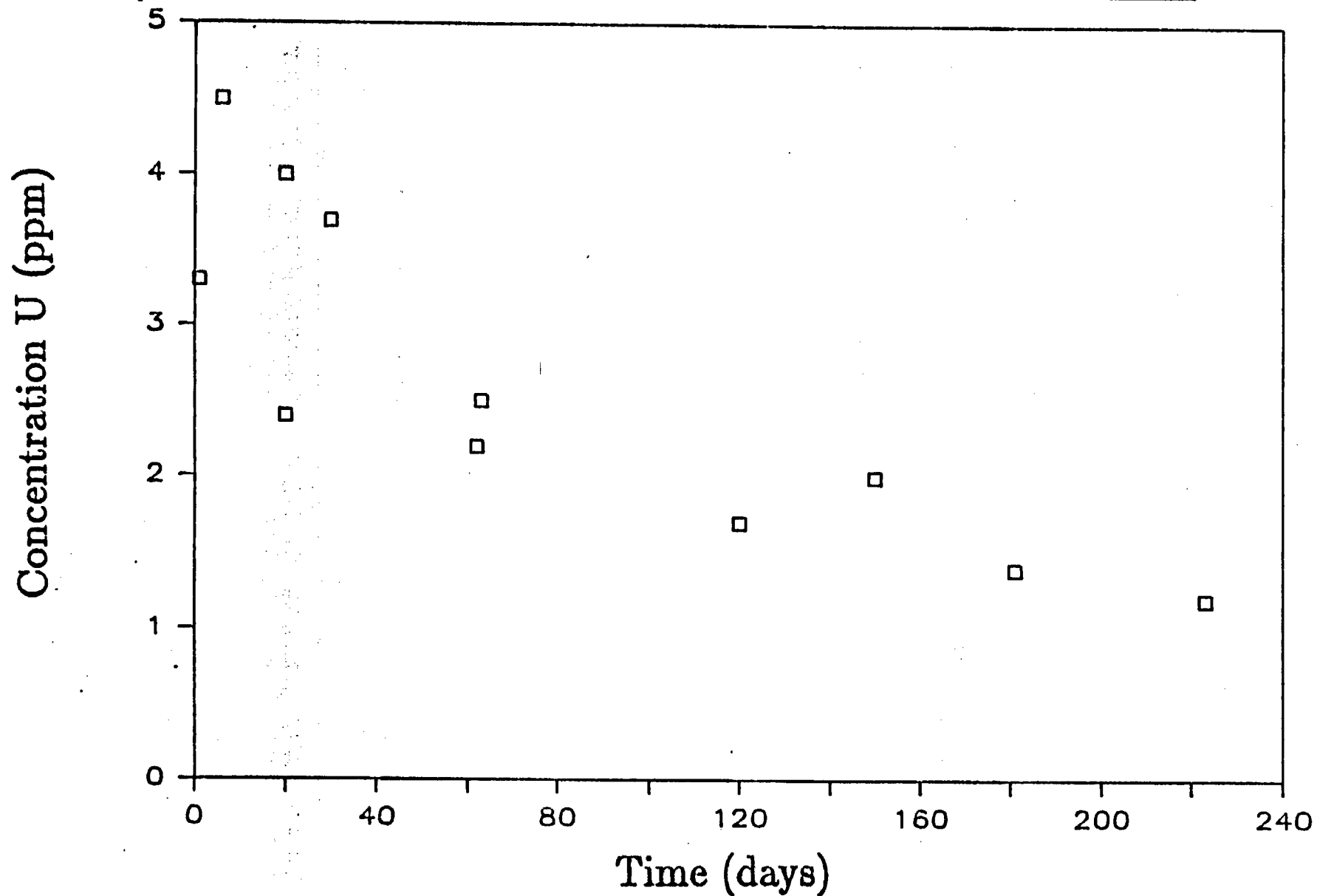
- Improper evaluation of experimental results.
- Solubility constants extracted from experimental data in which the solid phase was not identified.

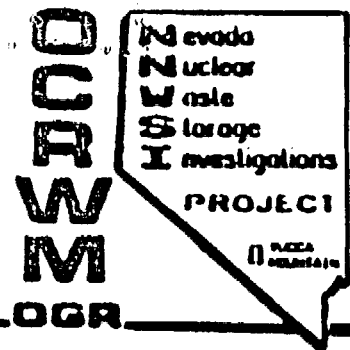
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PIZZA
MOUNTAIN

HEDL SPENT-FUEL DISSOLUTION STUDIES

J-13 + UO_2 (25°C, pH 8.1)

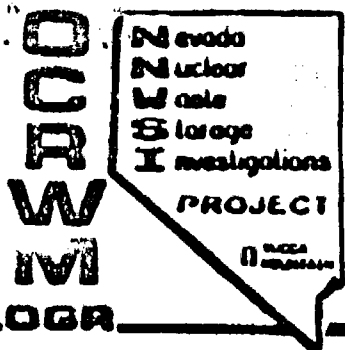


EQ3/6 DATABASE SUBSET = URANIUM (VI)

(Parks and Tripathi, 1985; This Study)

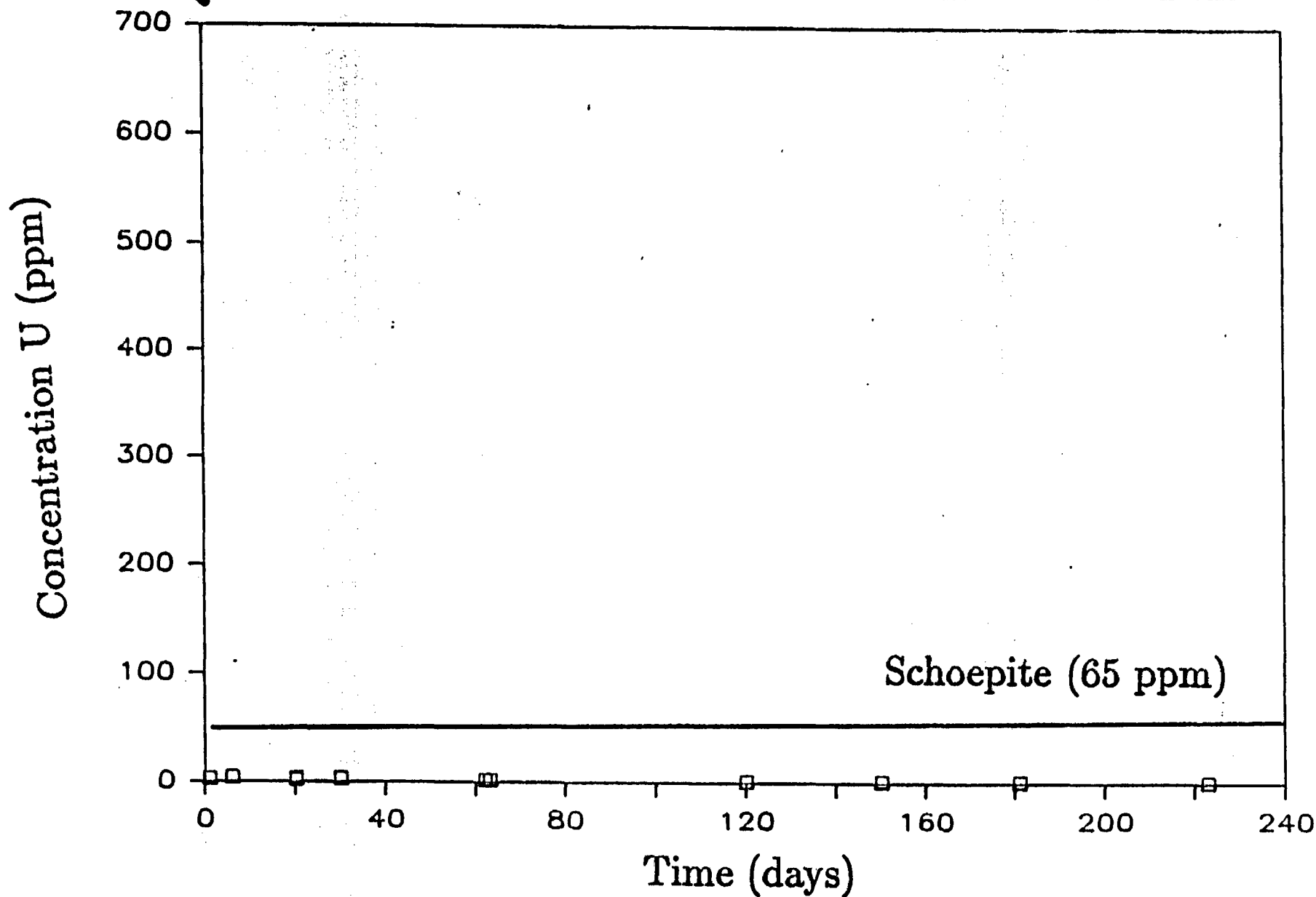


- 17 Aqueous Species Modified
- 5 Solids Modified
- 7 Species Added
- 5 Species Deleted



EQ3NR Solubility Constraint = Schoepite

J-13 + Uranium (25°C, pH 8.1)



EQ3/6 DATABASE SUBSET = URANYL SILICATES

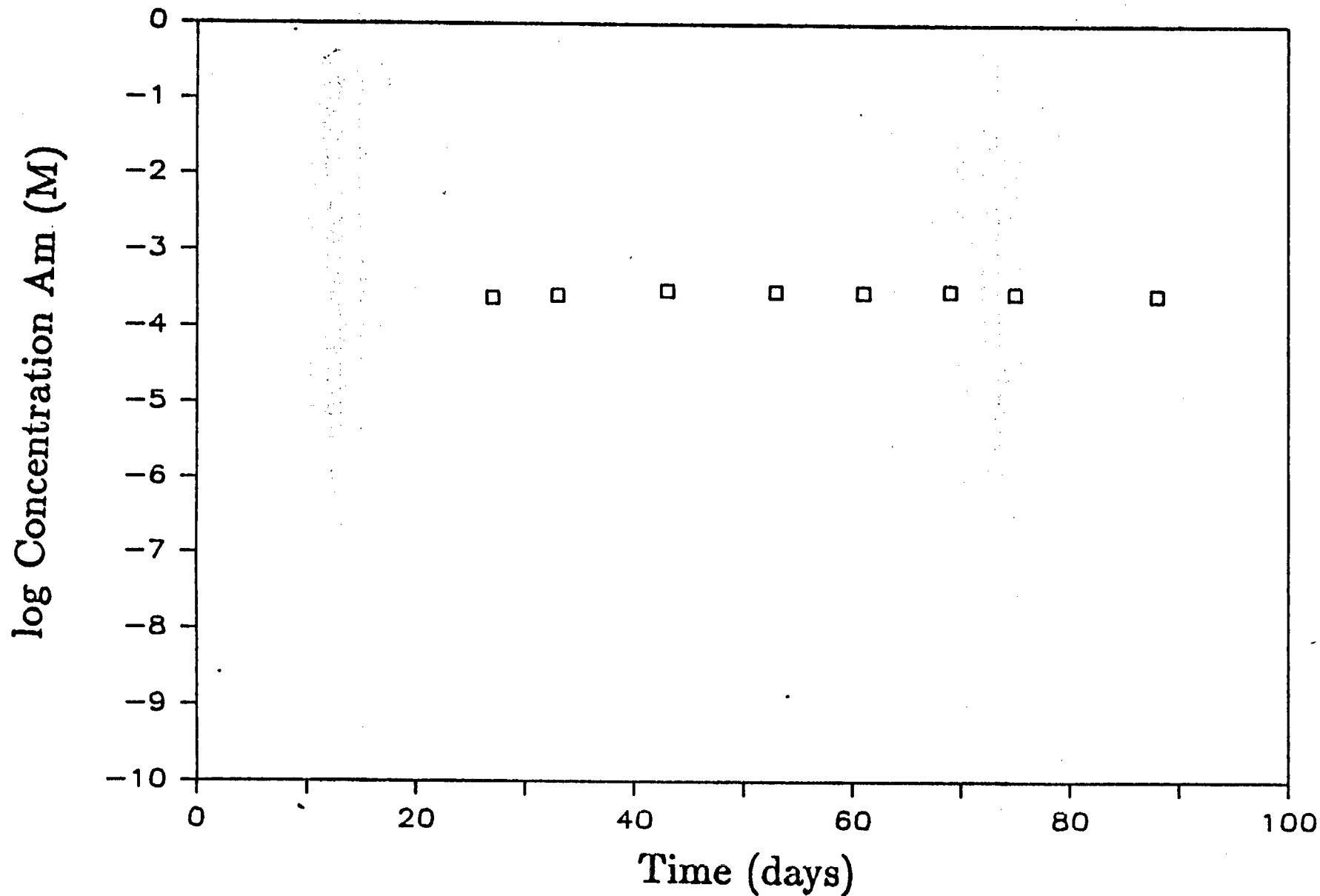
(Hemingway, 1982)



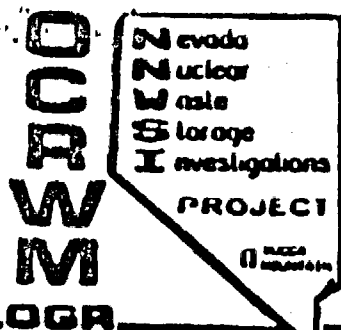
URANOPHANE	$\text{Ca}(\text{H}_3\text{O})_2(\text{UO}_2)_2(\text{SiO}_4)_2 \cdot 3\text{H}_2\text{O}$
BOLTWOODITE	$\text{K}(\text{H}_3\text{O})(\text{UO}_2)(\text{SiO}_4)$
Na BOLTWOODITE	$(\text{Na}_{.7}\text{Ca}_{.3})(\text{H}_3\text{O})(\text{UO}_2)(\text{SiO}_4) \cdot \text{H}_2\text{O}$
KASOLITE	$\text{Pb}(\text{UO}_2)(\text{SiO}_4) \cdot \text{H}_2\text{O}$
SKLODOWSKITE	$\text{Mg}(\text{H}_3\text{O})_2(\text{UO}_2)_2(\text{SiO}_4)_2 \cdot 2\text{H}_2\text{O}$
CUPROSKLODOWSKITE	$\text{Cu}(\text{UO}_2)_2(\text{SiO}_3\text{OH})_2 \cdot 6\text{H}_2\text{O}$
WEEKSITE	$\text{K}_2(\text{UO}_2)_2(\text{Si}_2\text{O}_5)_3 \cdot 4\text{H}_2\text{O}$
HAIWEEITE	$\text{Ca}(\text{UO}_2)_2(\text{Si}_2\text{O}_5)_3 \cdot 5\text{H}_2\text{O}$
SODDYITE	$(\text{UO}_2)_2(\text{SiO}_4) \cdot 2\text{H}_2\text{O}$

LBL Solubility Studies of Actinides

0.1 M NaClO₄ + ²⁴³Am³⁺ (25°C, pH 7)

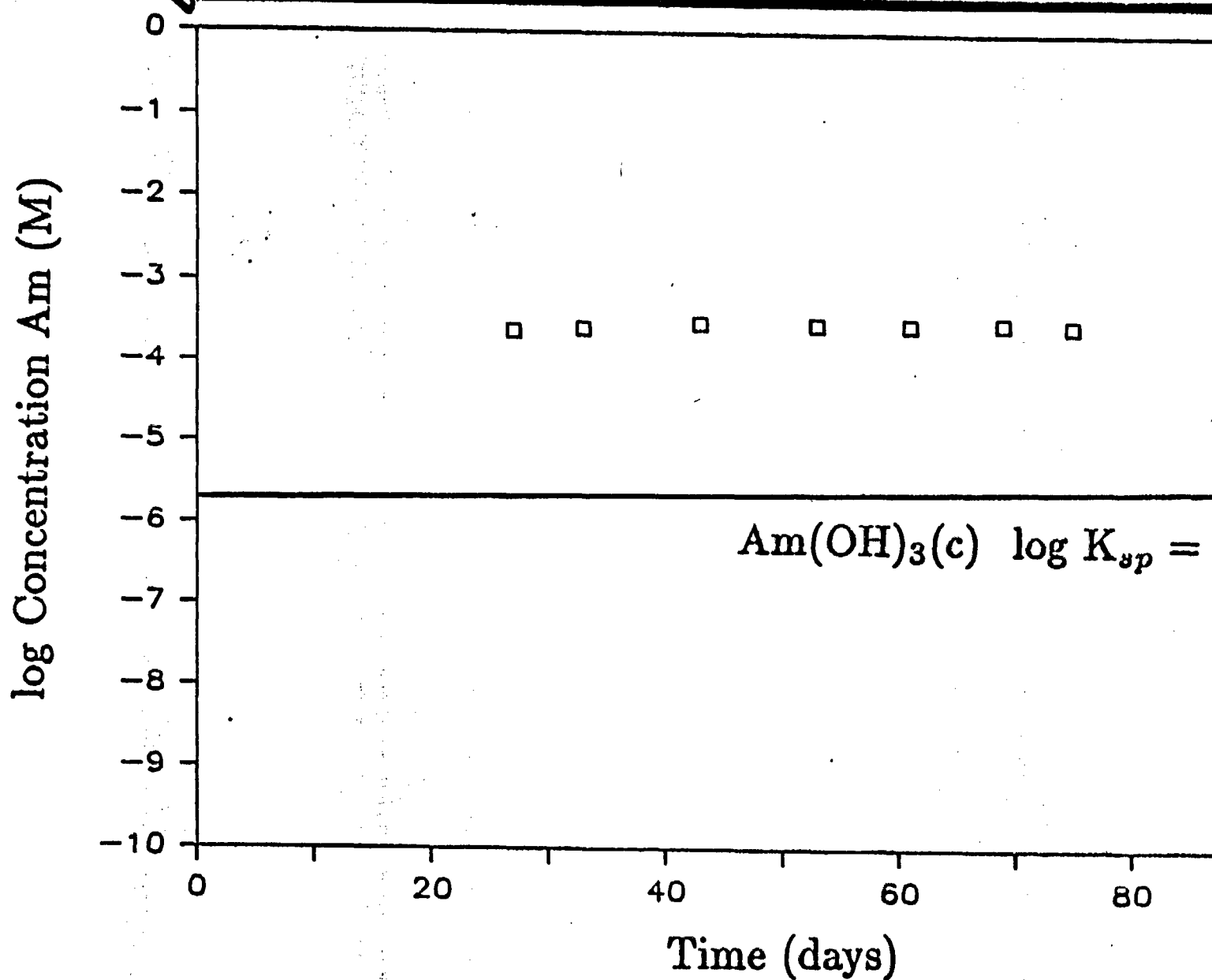


U.S. DEPARTMENT OF ENERGY



EQ3NR Solubility Constraint = $\text{Am}(\text{OH})_3(\text{c})$

0.1 M NaClO_4 + $^{243}\text{Am}^{3+}$ (25°C, pH 7)

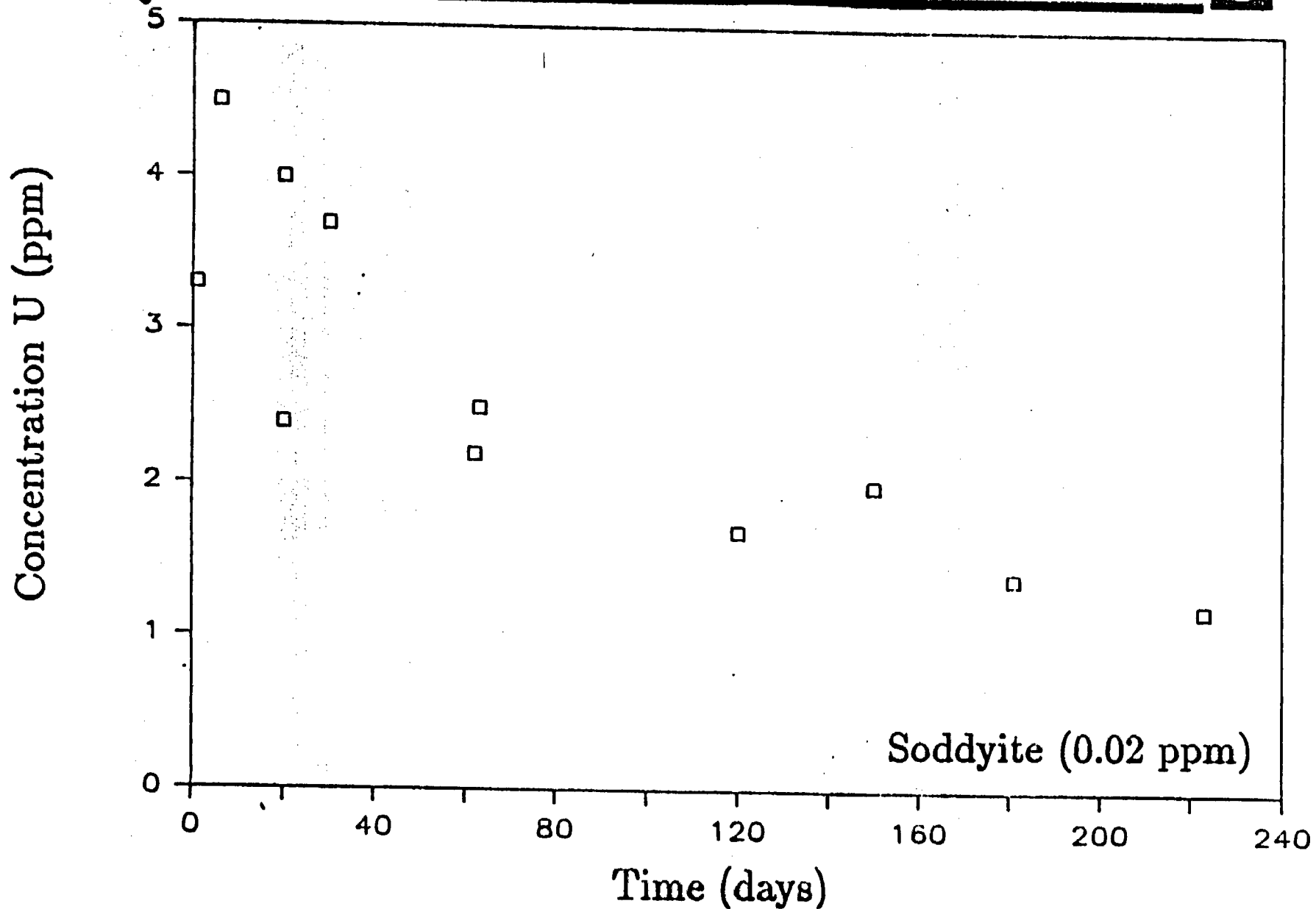


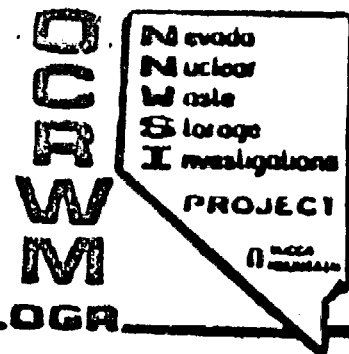
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EQ3NR Solubility Constraint = Soddyite

J-13 + Uranium (25°C, pH 8.1)



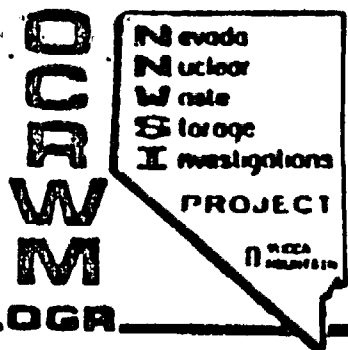


Summary

Future Needs



- Identification of uranium solid phases in dilute solutions.
- Thermodynamic and crystallographic data for uranyl silicate phases.
- Resolve inconsistencies in aqueous uranium (VI) carbonate system.

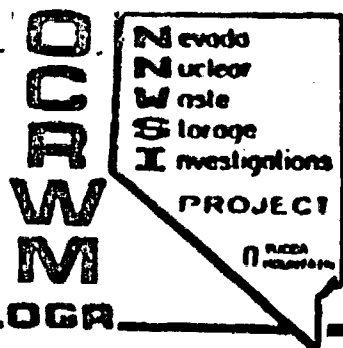


EQ3/6 DATABASE SUBSET = AMERICIUM

(Work in Progress, This Study)



- 6 Aqueous Species Modified
- 3 Solids Modified
- 2 Species Added
- 0 Species Deleted

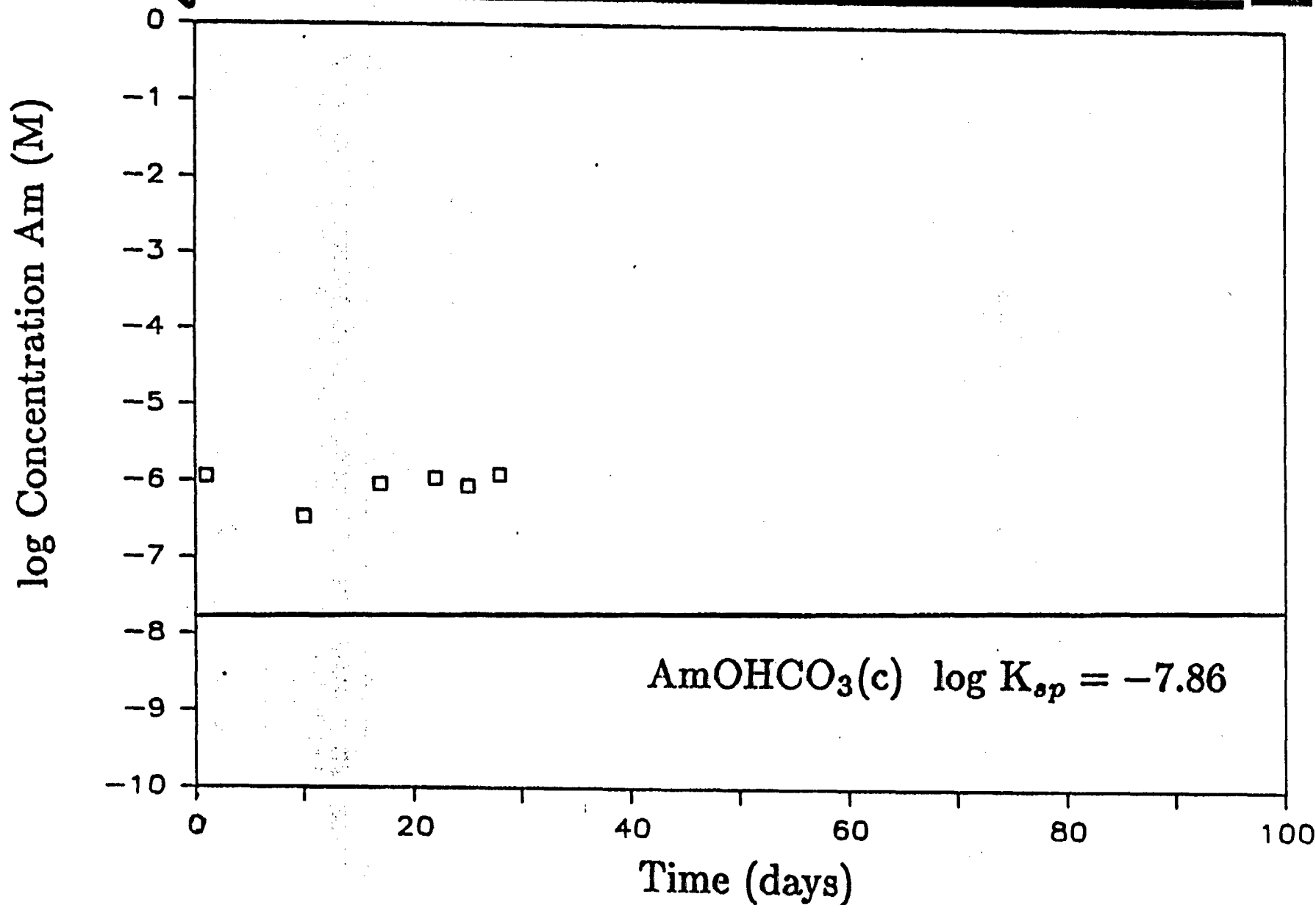


- Criteria Used to Revise Thermodynamic Data

- Evaluation of all experimental data in terms of a given set of solids and aqueous species.
- Give more weight to studies with aqueous complexes measured directly (potentiometric titration, solvent extraction).
- Give more weight to studies with solid reaction products identified by independent methods (xray, spectroscopy).
- If inconsistencies still exist among data values, conservative values are chosen to prevent underestimation.

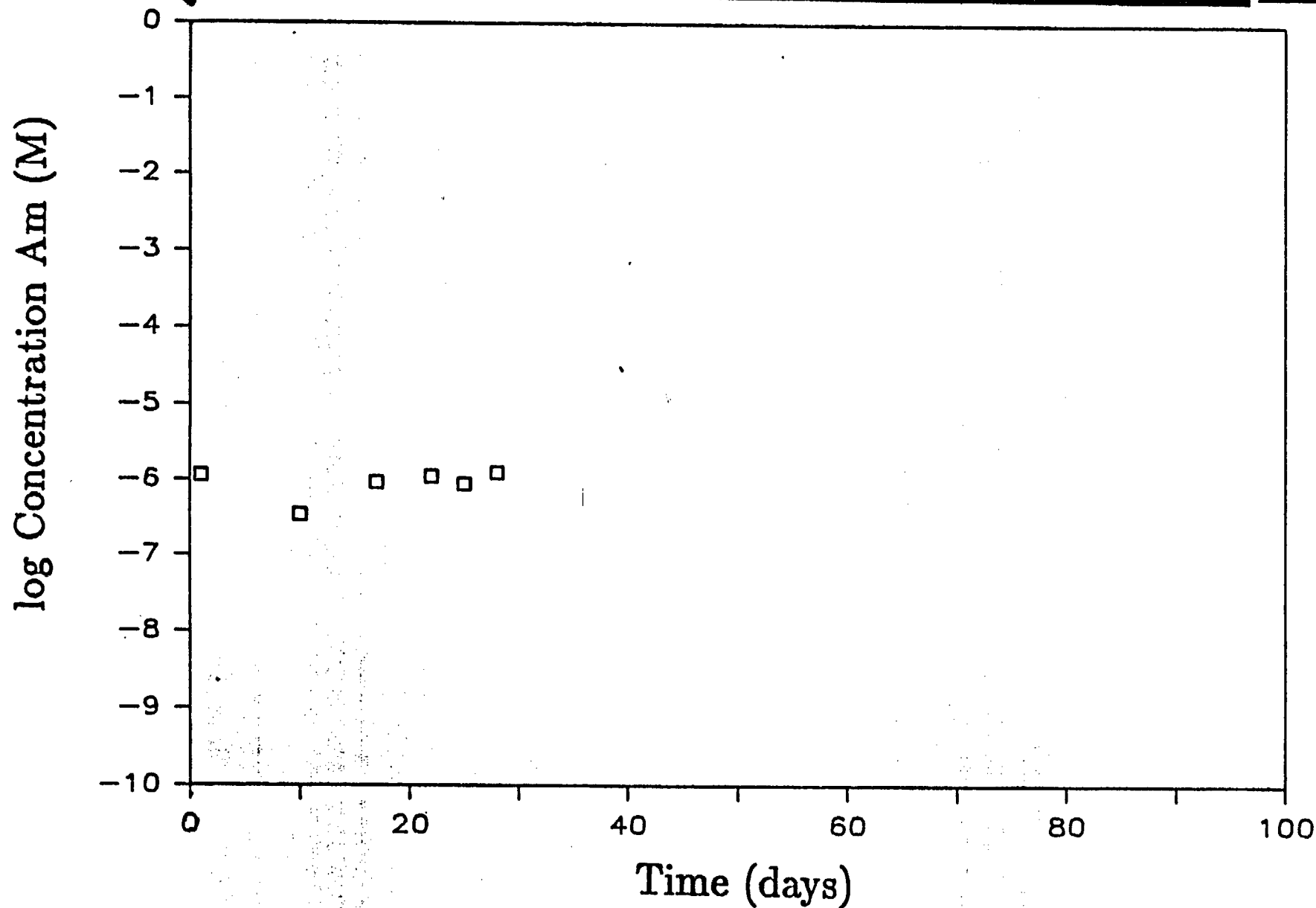
EQ3NR Solubility Constraint = $\text{Am}(\text{OH})\text{CO}_3(\text{c})$

J-13 + $^{243}\text{Am}^{3+}$ (25°C, pH 7)



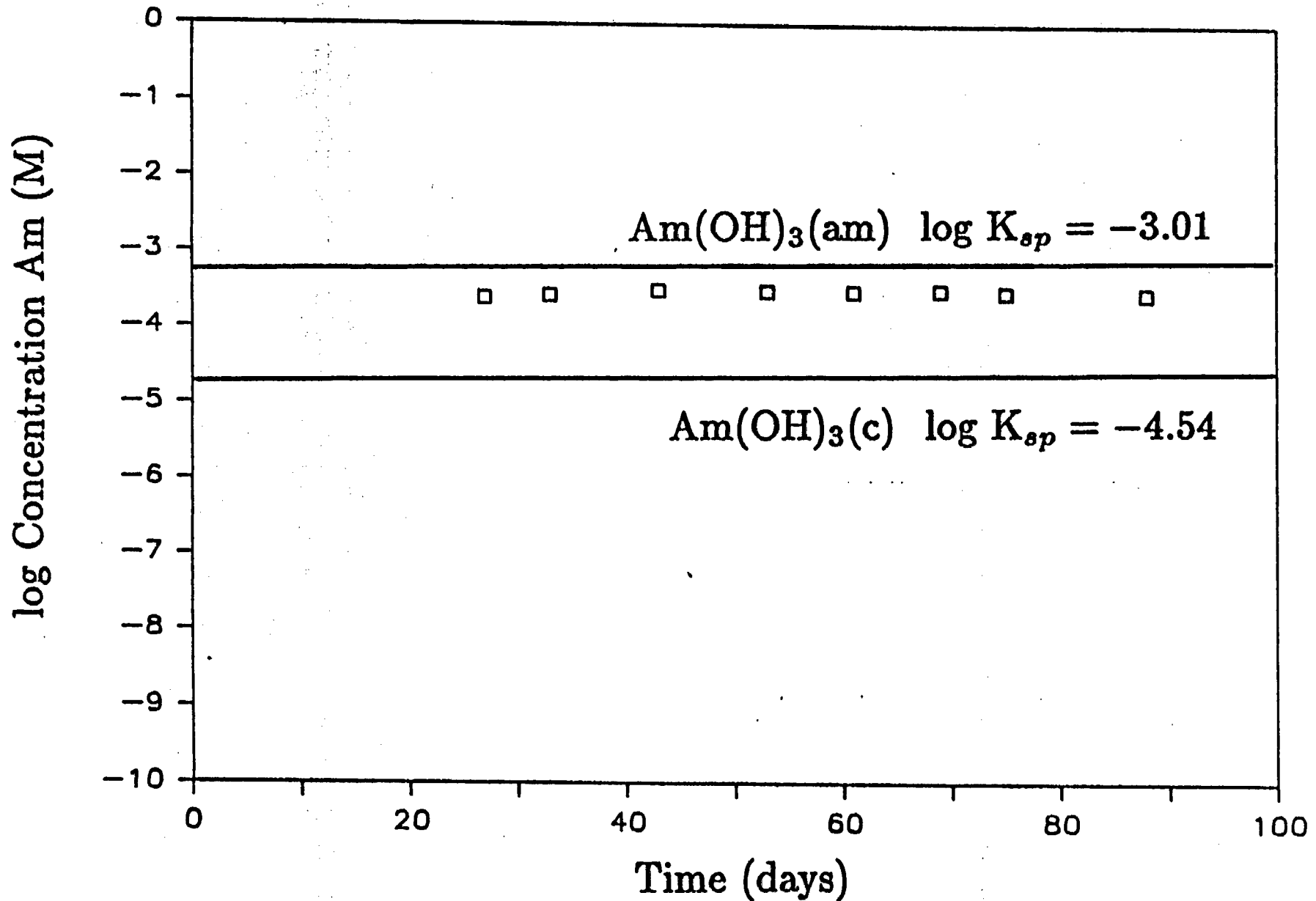
LBL Solubility Studies of Actinides

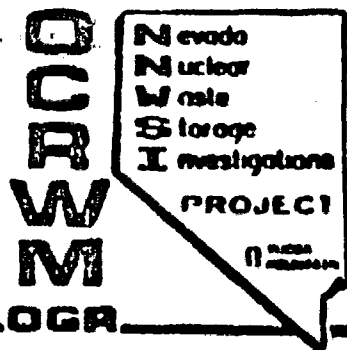
J-13 + $^{243}\text{Am}^{3+}$ (25°C, pH 7)



EQ3NR Solubility Constraint = $\text{Am}(\text{OH})_3(\text{am})$

0.1 M NaClO_4 + $^{243}\text{Am}^{3+}$ (25°C, pH 7)





Summary

Future Needs



- Additional experiments are needed in J-13 water to verify steady state concentrations have been reached.
- Resolve inconsistencies regarding chemistry of carbonate complexes at low concentrations.
- Further study of americium complexes in dilute groundwaters (bicarbonate, fluoride, sulfate).

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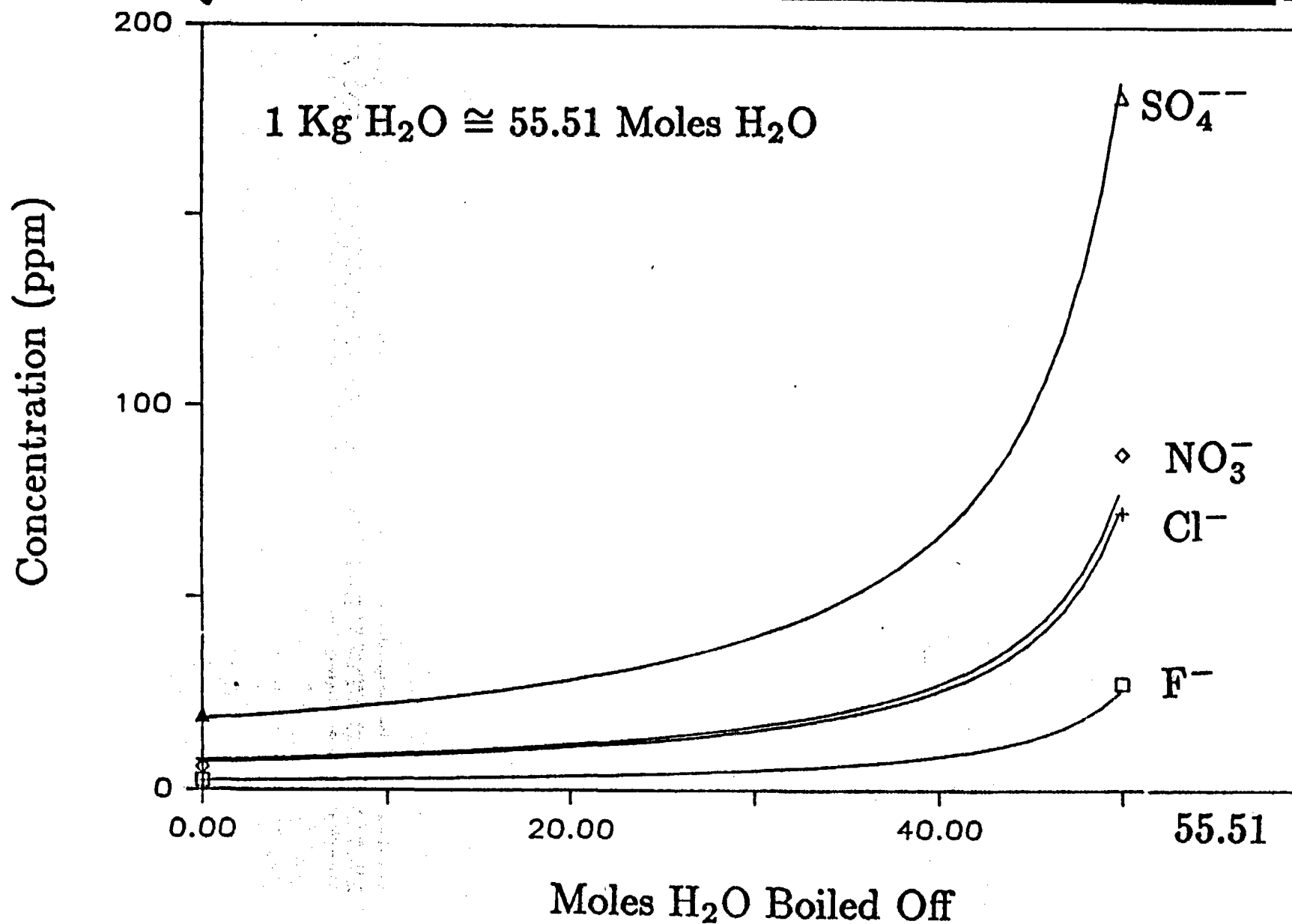
EQ6 APPLICATIONS

Concentration of J-13 as a Result of Boiling



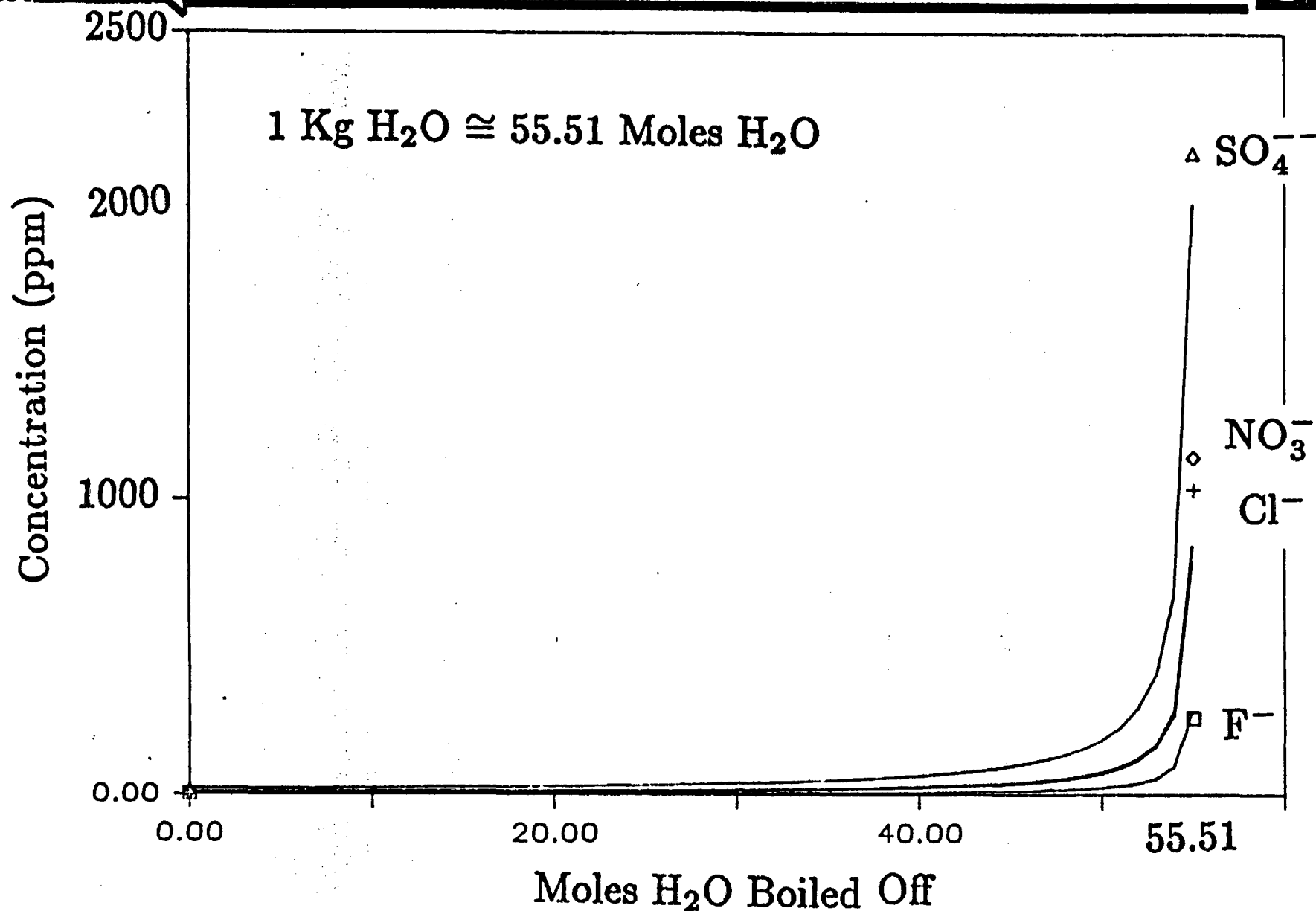
- Boiling is being investigated to help evaluate the effect of concentrated solutions in corrosion experiments.
- How well do EQ6 calculations match experimental anion concentrations for 10X and 100X solutions?

LLNL Concentrated J-13 Water 10X Anion Concentrations



LLNL Concentrated J-13 Water

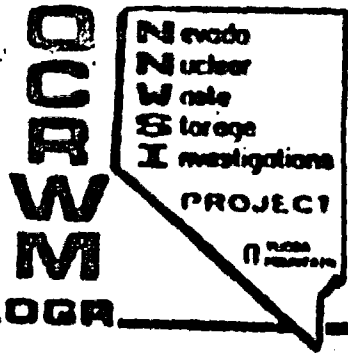
100X Anion Concentrations



Composition of Precipitate From 100X Solution



- Experimental Results (pH 9.8)
 - Ca-silicates
- EQ6 Simulation with CO₂ Loss (pH 10.01)
 - Calcite + Tremolite
 - Calcite + Tremolite + Quartz
- EQ6 Simulation without CO₂ Loss (pH 6.52)
 - Quartz + Talc + (Clay)
 - Clay + Quartz + Dolomite
 - Calcite + Fluorite + Muscovite

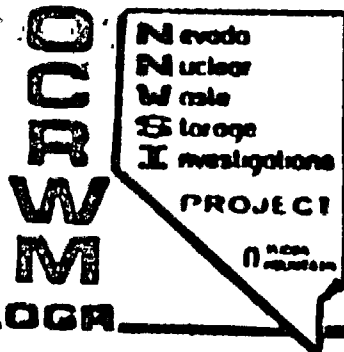


EQ6 APPLICATIONS

Water/Rock Simulations



- Concentrations of the major cation components in solution are compared with analytical results obtained from experiments.
- The precipitation of secondary phases predicted by EQ6 is compared with the alteration products observed on the core wafers after the experiments.

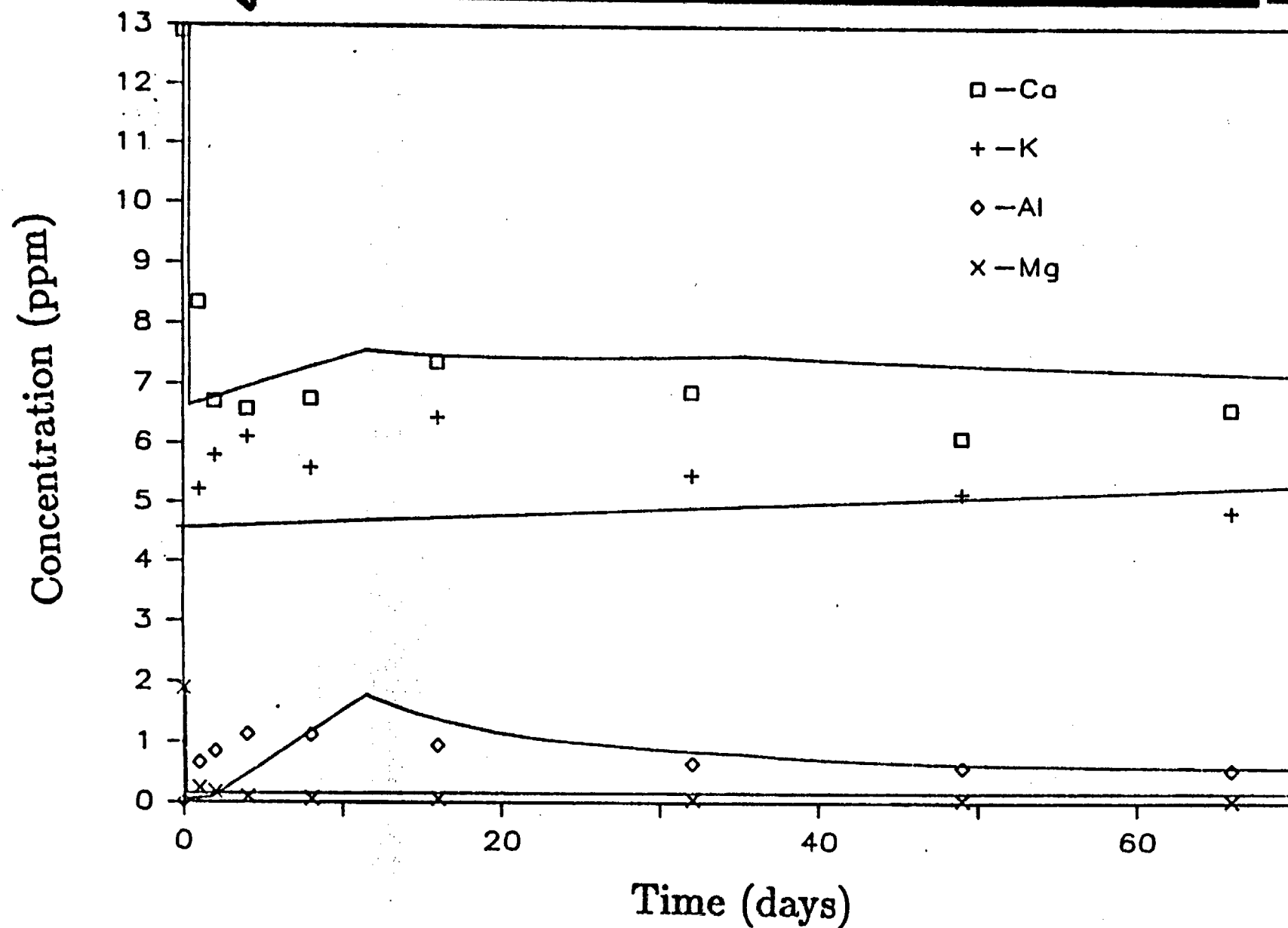


EQ6 Input for Each Reactant



- Name.
- Composition, if it is a solid solution.
- Amount.
- Initial surface area.
- Specify a rate law code and rate constants.

```
*-----
reactant= cristobalite
jcode= 0          jreac= 0
morr= 6.663e-02   modr= 0.
nsk= 1           sk= 16178.  fk= 0.2
nrk= 1
imech= 1
* rk from rimstidt and barnes (1980)- 180c
rk= 3.55e-13      ndact= 0          csigma= 1.
*-----
```



EQ6 Rock Recipe for Topopah Spring Tuff Core Wafer

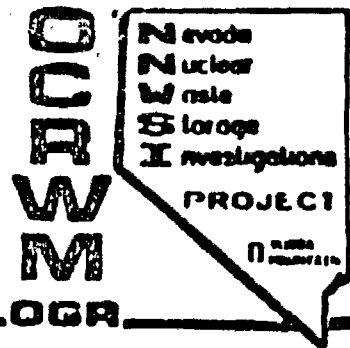


Phase	Weight Percent*	Moles of Reactant** (mole/gram)	(MORR)	Specific Surface Area+ (cm ² /g) (SK)	
Cristobalite	37.5	6.241 x 10 ⁻³	6.663 x 10 ⁻²	1516.2	16178.
Alkali Feldspar	43.14	1.587 x 10 ⁻³	1.694 x 10 ⁻²	1576.6	16822.
Quartz	16.9	2.813 x 10 ⁻³	3.003 x 10 ⁻²	602.5	6429.
Plagioclase	1.13	4.246 x 10 ⁻⁵	4.533 x 10 ⁻⁴	40.45	432.
Mg-beidellite	1.21	3.301 x 10 ⁻⁵	3.522 x 10 ⁻⁴	40.45	432.
Biotite	0.13	2.759 x 10 ⁻⁶	2.946 x 10 ⁻⁵	3.8	40.5

* Bulk Density = 2.335 g/cm³.

** Mass of Core Wafer = 2.2496 g, sample volume= 210.7 g.

+ BET Ar surface area = .378 m²/g.



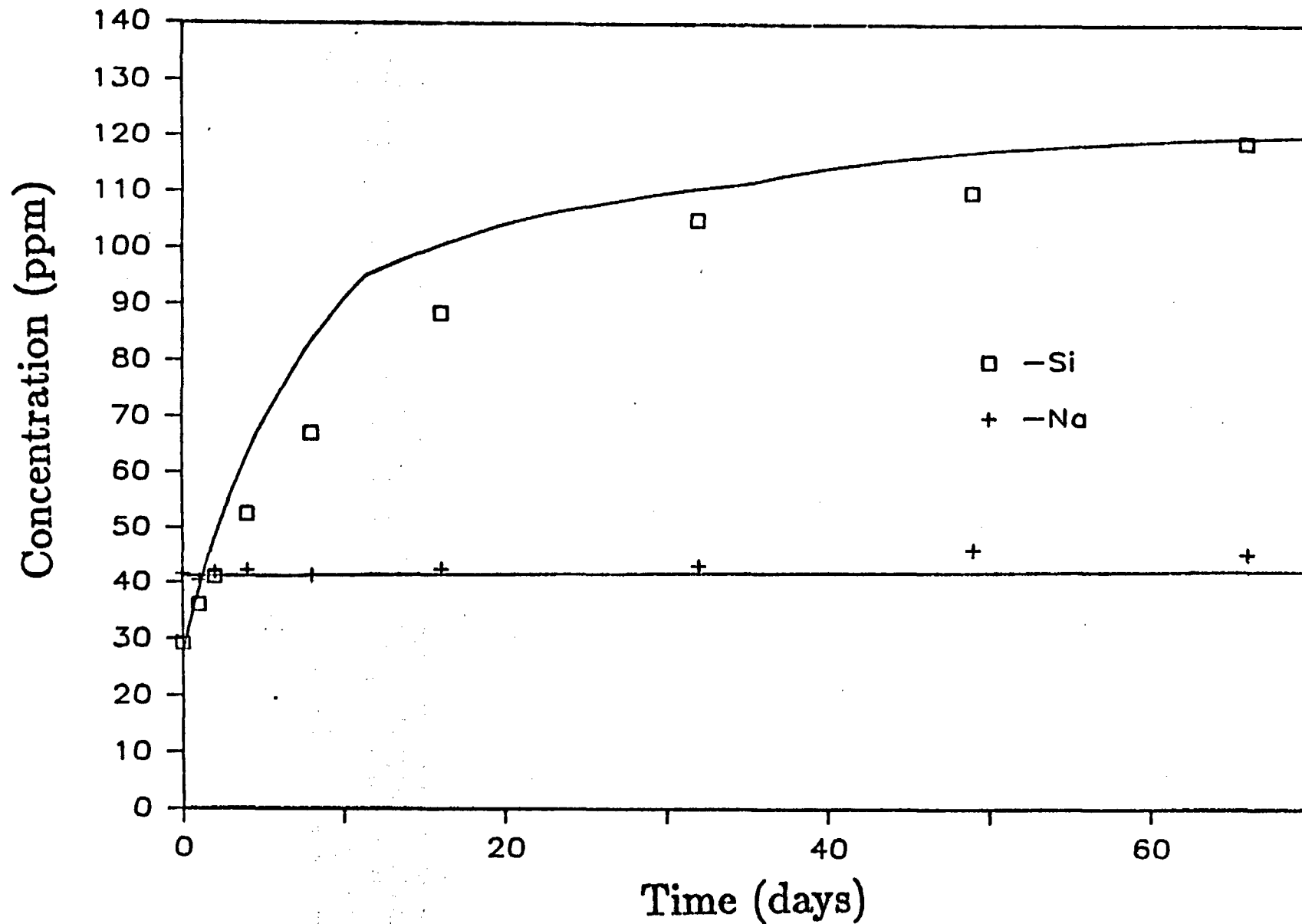
Compositional Analysis of Topopah Spring Tuff



Phase	Composition	Volume Percent
Cristobalite	SiO ₂	44
Alkali Feldspar	Or.58Ab.41An.01	39
Quartz	SiO ₂	14.9
Plagioclase	Or.07Ab.76An.17	1
Mg-beidellite	Mg.165Al _{2.33} Si _{3.67} O ₁₀ (OH) ₂	1
Biotite	Phlog.43Ann.57	0.1
TOTAL		100.0

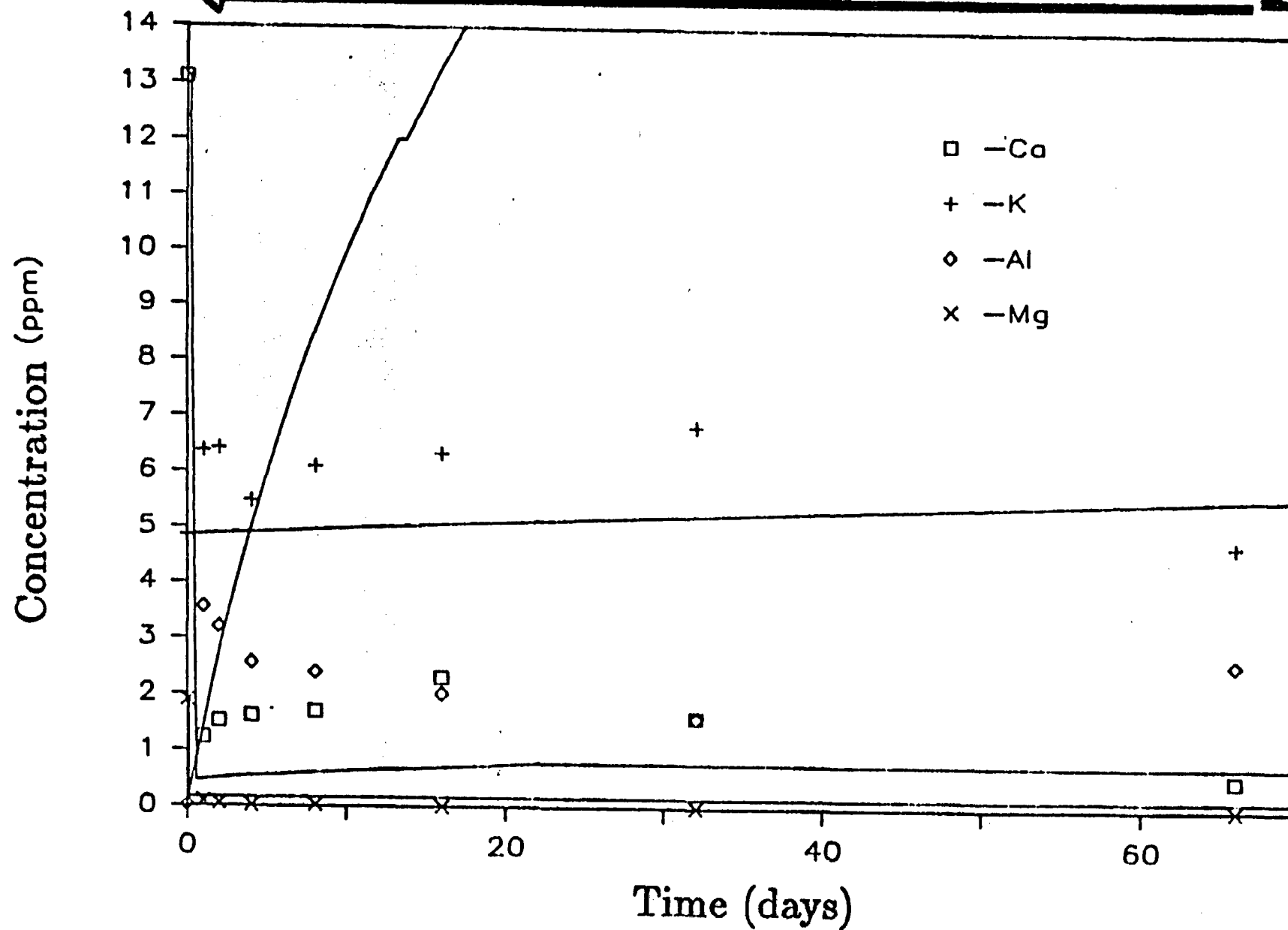
150°C Solution Compositions

EQ6 Simulation



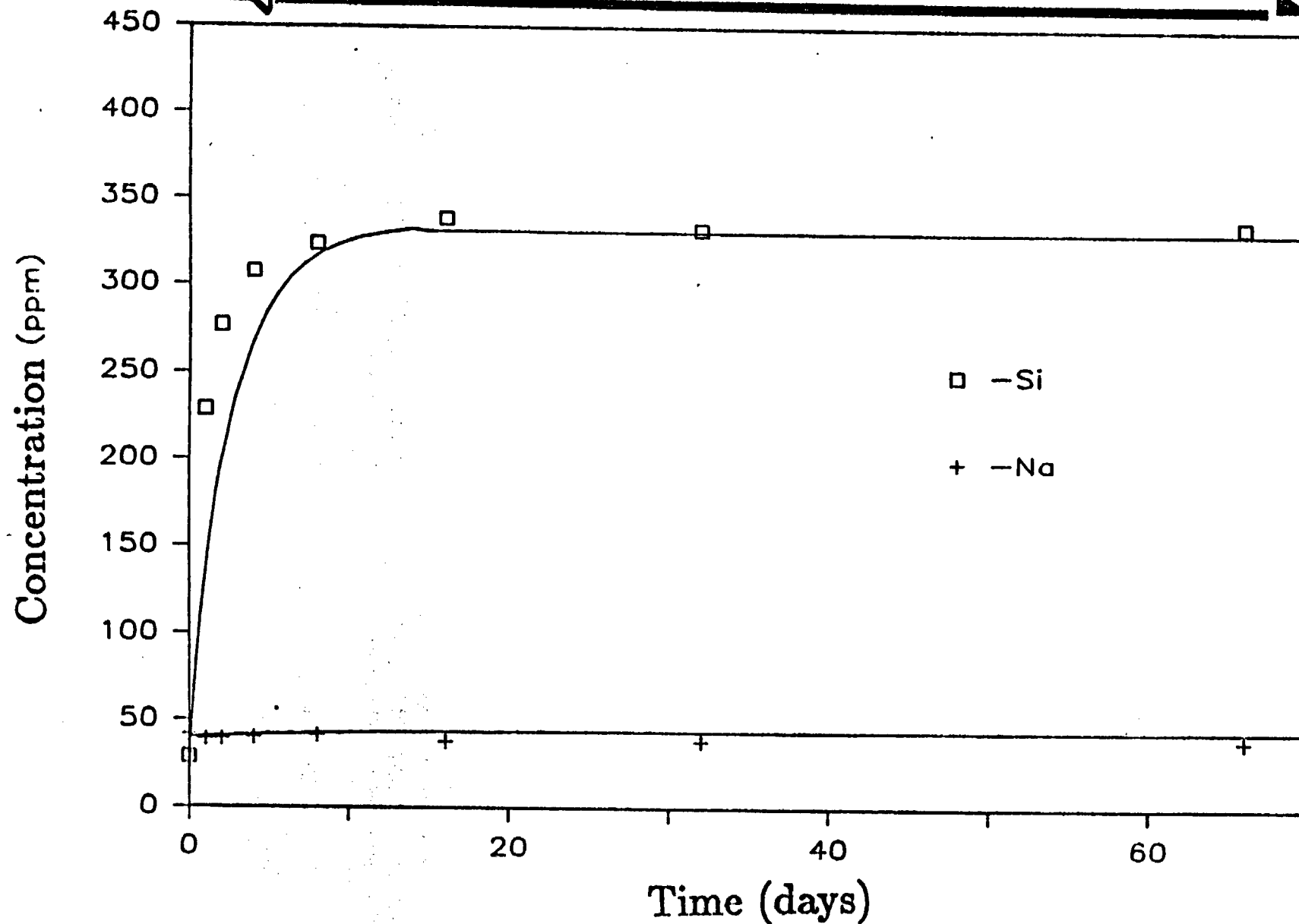
250°C Solution Compositions

EQ6 Simulation



250°C Solution Compositions

EQ6 Simulation



Secondary Mineral

Identified on Surfaces of Reacted Core Wafers



- Dachiardite



- Experimental Conditions:

Long Term 150°C Experiments (≈ 300 days).

Short Term 250°C Experiments (≈ 70 days).

EQ3/6 DATABASE SUBSET = ZEOLITES



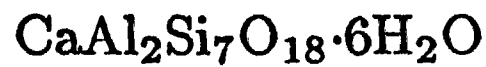
ANALCIME



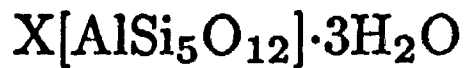
WAIRAKITE



HEULANDITE



MORDENITE

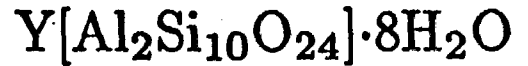


X = Na, K

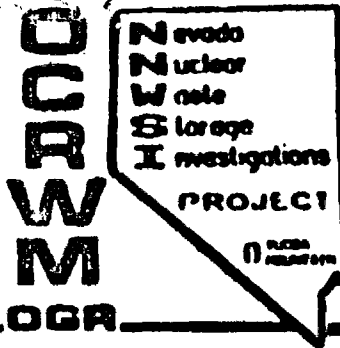
CLINOPTILOLITE



X = Na, K



Y = Ca, Mg



Summary of EQ6 Tpt Tuff + J-13 Simulations



- Solution trends suggest that EQ6 can nearly match experimental data for short simulations at 150°C.
- Data base limitations severely handicap successful simulations for long term 150°C and 250°C experiments.
- Additional thermodynamic data is needed for zeolite compositions.

Bechtel National, Inc.

Engineers - Constructors



Fifty Beale Street

San Francisco, California

Mail Address: P.O. Box 3965 San Francisco, CA 94119

July 15, 1985

BSL-086-17299

C. V. Subramanian
Sandia National Laboratories
Division 6311
P.O. Box 5800
Albuquerque, New Mexico 87185

Subject: Seismic/Tectonic Position Paper Draft Definitions
(Section 3.2.2)

Reference: Letter, M.D. Voegele to D.L. Vieth, "Seismic Tectonic
Working Group Meeting Minutes, dated June 28, 1985
(L85-RC-MDV-84)

Dear Subra,

Attached is a set of draft definitions as required for Bechtel action
in the reference letter and meeting minutes.

Very truly yours,

Neil A. Norman
for Neil A. Norman, PE
Project Manager

NAN:LJJ:js

Enclosures

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SEISMIC DEFINITIONS

ACCESSIBLE ENVIRONMENT - "Means: (a) the atmosphere; (2) land surfaces; (3) surface waters; (4) oceans; and (5) portions of the lithosphere that are beyond the controlled area." (40 CFR 191)

ACTIVE FAULT - "A fault on which offset at the ground surface, or at the near-surface depths of the geologic repository, is an anticipated event on the basis of historical, seismological, or geologic evidence. The surface or near-surface offset will generally be accompanied by an earthquake of magnitude greater than 5."

ALTERNATE DEFINITIONS: "An active fault is a fault that has slipped in historic or recent geologic time, and is likely to have renewed displacements in the future. The fault activity is indicated by historic, geologic, or geophysical evidence and may occur at rates that vary from very low, with long recurrence intervals, to very high, with very short recurrence intervals..." (Slemmons, U.S. Army Corps Of Eng. Misc. Paper S-73-1, No. 6, 1977). "A fault that on the basis of historical, seismological, or geological evidence has a high probability of producing an earthquake" (Shah, et al., "Earthquake Spectra", Vol. 1, No. 1, 1984).

COMMENTARY: The definition in 10 CFR 960.2 is taken from the "Glossary of Geology" of the Amer. Geol. Inst. (1972). It is unsatisfactory because it merely requires recurrent movement on the fault without any indication of recency of last movement. Therefore, any fault that has been offset twice could be considered active. The "surface" (or repository depth) and "anticipated" provisions of the suggested definition attempt to tie a fault's activity directly to design and licensing concerns.

ANALYTICAL MODEL - "A mathematical representation of physical phenomena that is amenable to closed-form (analytical) solution (i.e., the governing equation and associated boundary conditions have an exact solution)." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

ANTICIPATED EVENT - "Those natural processes and events that are reasonably likely to occur during the period the intended performance objective must be achieved. To the extent reasonable in the light of the geologic record, it shall be assumed that those processes operating in the geologic setting during the Quaternary Period continue to operate but with the perturbations caused by the presence of emplaced radioactive waste superimposed thereon." (10 CFR 60)

AQUIFER - "A formation, a group of formations, or a part of a formation, that contains sufficient saturated permeable material to yield significant quantities of water to wells. Aquifers may be classified as confined or unconfined depending on the presence or absence of a water table." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater," 1979).

BENCHMARKING - "The process of comparing the results obtained by different mathematical models to ensure that the codes are error-free." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

BOUNDARY CONDITIONS - "Conditions that must be satisfied by the solution of a differential equation for given values of the independent variables (e.g., specific values of the pressure head are assigned at given points in space.)." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

CALIBRATION - "The process of comparing the values calculated by a mathematical model with the measured values." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

CANDIDATE AREA - "An area, within a geohydrologic setting, that is recommended by the Secretary of Energy under Section 112 of the Act for site characterization, approved by the President under Section 112 of the Act for characterization, or undergoing site characterization under Section 113 of the Act." (10 CFR 960)

CAPILLARY FRINGE - "Zone above the water table that is saturated or nearly saturated, and where the pressure is less than atmospheric. Also referred to as tension-saturated zone." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

CLASS I STRUCTURE - "Any structure, system, or component means an item whose failure would result in a consequence exceeding the limits and criteria specified in 10 CFR 60 for protection of the public during preclosure and postclosure periods." (SNL/BNI)

CLASS II STRUCTURE -

To be determined

CLASS III STRUCTURE -

To be determined

CONCEPTUAL MODEL - "A description of the domain of interest and the physical phenomena involved in a manner that is sufficiently detailed to be scientifically defensible, yet simple enough to be amenable to mathematical representation." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

CONFINED AQUIFER - "An aquifer bounded above and below by relatively impervious materials (confining units)." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

CONSERVATISM - "An approach leading to the selection of assumptions and parameters that tend to overestimate the severity of potentially adverse events." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

CONTROLLED AREA - "A surface location, to be identified by passive institutional controls that prohibit incompatible activities, extending horizontally no more than two kilometers in any direction from the outer boundary of the original location of the radioactive wastes in a disposal system, and the subsurface underlying such a surface location." (40 CFR 191)

COMPLEMENTARY CUMULATIVE DISTRIBUTION FUNCTION (CCDF) - "Represents the probability that releases to the accessible environment will be equal to or greater than a given value. It is developed by subtracting each probability value of the cumulative distribution function (CDF) from 1.0. The CDF represents the probability that releases to the accessible environment will be less than or equal to a given value. The CDF is developed by integrating the probability density function representing releases; the CDF includes uncertainties." (SNL/BNI)

DELPHI TECHNIQUES - "A methodology for reducing the uncertainty attached to parameters, phenomena, or events, based on independent expert opinions." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

DESIGN EARTHQUAKE 1 - "A severe earthquake motion for use in evaluating and designing facilities. The ground motion is that expected at the site with a return period of 2000 years as evaluated from an appropriate probabilistic model of the seismicity and tectonics of the site region."

ALTERNATE DEFINITION: "A specification of the seismic ground motion at a site; used for the earthquake-resistant design of a structure, system or component." (Shah, et al., "Earthquake Spectra", Vol. 1, No. 1, 1984).

COMMENTARY: The first definition is essentially that of SAND85-7104 (Blume, 1985). Some issues may need further consideration such as the appropriate return period for this earthquake, its characterization as severe when this is not necessarily the case for a 2000 year ground motion, and a better idea of what constitutes an "appropriate" probabilistic model.

DESIGN EARTHQUAKE 2 - "A moderate earthquake motion for use in evaluating and designing facilities. The ground motion is that expected at the site with a return period of 500 years using the same probabilistic model of site region seismicity and tectonics." (SAND85-7104, Blume, 1985)

DESIGN EVENT - "An occurrence which needs to be considered in system and installation design. It can be classified according to its expected frequency of occurrence, and when so classified, used in conjunction with objectives associated with maintenance of system capability to provide a logical and systematic approach to protection by design." (ANSI/ANS-57.9-1984)

ALTERNATE DEFINITIONS: (1) "A tectonic or seismic process or event with a reasonable potential for occurrence and one that, should it occur, might affect radiological containment requirements of facility operation or disposal systems. It is an event that should be

considered in evaluating regulatory compliance of the repository."

(2) "A specification of one or more earthquake source parameters, and of the energy release with respect to the site of interest; used for the earthquake-resistant design of a structure." (Shah, et al., "Earthquake Spectra", Vol. 1, No. 1)

COMMENTARY: The alternative definition (1) basically adopts the intent of a "process and event" to be considered in a "performance assessment" and attempts to expand it to include the operational phase of the repository. The possible alternative concept of a maximum design event in a deterministic process is not suggested here, although it could be. Preliminary review of the applicable regulations did not reveal the use of this term.

DESIGN GROUND MOTION - "A dynamic vibratory ground motion design event."

COMMENTARY: This is a particular example of a design event and the same comments apply.

DESIGN SEISMIC EVENTS - "A specification of one or more earthquake source parameters, and of the location of energy release with respect to the site of interest; used for the earthquake-resistant design of a structure." (Earthquake Spectra, 1-1, 11/84, pg. 33)

DESIGN SPECTRA - "A representation of a design ground motion as the maximum response to that ground motion of a single-degree-of-freedom, damped harmonic oscillator for various oscillator natural frequencies. This is a common design tool for the analysis of free-standing structures."

ALTERNATIVE DEFINITION: "A set of curves for design purposes that gives acceleration, velocity, or displacement (usually absolute acceleration, relative velocity, and relative displacement of the vibrating mass) as a function of period of vibration and damping." (Shah, et al., "Earthquake Spectra", Vol. 1, No. 1, 1984)

COMMENTARY: Many alternative definitions exist for this concept, which is largely divorced from licensing interpretation.

DESIGN UNDERGROUND NUCLEAR EXPLOSION 1 - "A severe UNE motion for use in evaluating and designing facilities. The DUNE-1 ground motion is that expected at the site with a return period of 2000 years as evaluated from an appropriate probabilistic model of future weapons testing at the Nevada Test Site (NTS)."

COMMENTARY: This definition is, again, essentially that of SAND85-7104 except Class I has been removed. Issues, again, perhaps requiring further examination exist. In particular, what is an appropriate probabilistic treatment of a phenomenon completely under human control?

DESIGN UNDERGROUND NUCLEAR EXPLOSION 2 - "A moderate UNE motion for use in evaluating and designing facilities. The DUNE-2 ground motion is that expected at the site with a return period of 500 years as evaluated using the same probabilistic model of future weapons testing."

COMMENTARY: Comments similar to those for the DUNE-1 apply.

DETERMINISTIC - "Refers to the types of mathematical formulations wherein physical parameters, stresses, or boundary conditions are considered uniquely determined at a given point in time and space." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

DETERMINISTIC ANALYSIS - "An analysis derived largely from estimates and judgment of a recognized expert in the specific field of analysis." (SNL/BNI)

ALTERNATIVE DEFINITION: "A method to estimate the maximum potential earthquake ground motion reasonably expected at a site on the basis of a characterization of the site region as containing certain geologic structures capable of causing earthquakes of some maximum magnitude or as made up of certain seismogenic provinces. Sizes and distances of earthquakes associated with structures and provinces are considered but the distributions of earthquakes in time and by magnitude are ignored."

COMMENTARY: This is the type of analysis required for 10 CFR 100 Appendix A, and this, perhaps, may be made a part of the definition. It leads to the SSE but this was not noted because it would require another definition not relevant to the waste disposal licensing process.

DISTRIBUTION COEFFICIENT - "A measure of radionuclide adsorption by the geologic media, expressed as the ratio of the mass of solids on the solid phase per unit mass of the solid phase, to the concentration of solids in solution. Distribution and retardation coefficients are linearly related." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

DISTURBED ZONE - "That portion of the controlled area, excluding shafts, whose physical or chemical properties are predicted to change as a result of underground facility construction or heat generated by the emplaced radioactive waste such that the resultant change of properties could have a significant effect on the performance of the geologic repository." (10 CFR 960)

EFFECTIVE POROSITY - "A measure of interconnected pore space available for the transmission of fluids, expressed as the ratio of interconnected pores or fracture openings to the volume of intact rock." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

EXCEEDENCE PROBABILITY - "The probability that an event will occur during a specific exposure time. For seismic events, "exceedence probability" means the probability that a specified level of ground motion or specified social or economic consequences of earthquakes, will be exceeded at a site or in a region during a specified exposure time." (Shah, et al., "Earthquake Spectra", Vol. 1, No. 1, 1984)

EXPECTED REPOSITORY PERFORMANCE - "The manner in which the repository is predicted to function, considering those conditions, processes, and events that are likely to prevail or may occur during the time period of interest." (10 CFR 960)

FAULT - "A fracture or zone of fractures along which there has been displacement, parallel to the fracture zone, of the sides relative to one another. The amount of displacement may be from a few centimeters to a few kilometers or more."

COMMENTARY: The definition in 10 CFR 960.2 is taken from "Dictionary of Geological Terms" of the Amer. Geol. Inst. 91062), except "side" should be "sides" and the idea of displacement of "a few inches or many miles" has been omitted.

GEOHYDROLOGIC SYSTEM - "The system of geohydrologic units, including recharge and discharge areas, and interconnection between units." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

COMMENTARY: This definition is different from 10 CFR⁹⁶⁰ in that the natural or man-induced processes or events that could affect ground-water flow are not considered part of the geohydrologic system; rather these are stresses upon this system.

GEOHYDROLOGIC UNIT - "Aquifer, aquiclude, or combination thereof forming a reasonably distinct portion of the geohydrologic system." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

GEOLOGIC SETTING - "The geologic, hydrologic, and geochemical properties of the repository site region. The portion of the geologic setting that provides isolation of the radioactive waste makes up part of the geologic repository."

COMMENTARY: The above is a paraphrase of the 10 CFR 60 definition with the addition of the second sentence from 60.113. The concept is importantly of licensing as well as geotechnical content.

GROUND WATER - "All subsurface water, as distinct from surface water." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

GROUND-WATER FLUX - Rate of ground-water flow per unit area of the porous or fractured media, measured perpendicular to the flow direction. (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

GROUND-WATER SOURCES - "Aquifers that have been or could be, in the foreseeable future, technologically and economically developed as sources of water." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

GROUND-WATER TRAVEL TIME - "The time required for a unit volume of ground water to travel between two locations. It is equal to the length of the flow path divided by the ground-water velocity." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

COMMENTARY: This definition is similar to that of 10 CFR 960 except that (1) velocity has been defined separately, and (2) the last sentence - considered self-explanatory - was deleted.

HYDRAULIC CONDUCTIVITY - "A measure of the ability of subsurface materials to conduct water. Hydraulic conductivity is a function of the geologic materials properties and the fluid properties. It is equal to the volume of water moving through a unit area normal to the flow direction, per unit time, and under a unit hydraulic gradient." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

HYDROLOGIC PROCESS - "A hydrologic phenomenon that exhibits continuous changes over time, whether slow or rapid." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

HYDROLOGIC PROPERTIES - "The properties of a geohydrologic unit that characterize its ability to hold and transmit water. These include hydraulic conductivity or transmissivity, porosity, effective porosity, and storage coefficient or specific yield." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

IMPORTANT TO SAFETY - "Reference to structures, systems, and components means those engineered structures, systems, and components essential to the prevention or mitigation of an accident that could result in a radiation dose to the whole body, or any organ, of 0.5 rem or greater at or beyond the nearest boundary of the unrestricted area at any time until the completion of permanent closure." (10 CFR 60)

INITIAL CONDITIONS - "Conditions that must be satisfied by the solution of the differential equation at the origin of the time interval under consideration." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

LIKELY CONSEQUENCE OF FAILURE - "Processing or displaying the qualities, characteristics, or attributes that provide a reasonable basis for confidence that what is expected indeed exists or will occur." (10 CFR 960)

MATHEMATICAL MODEL - "The set of equations and associated boundary conditions that represent in a mathematical form the physical phenomena qualitatively described by a conceptual model. A mathematical model can be either analytical or numerical." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

MAXIMUM CONSEQUENCE OF FAILURE - "The estimate of the maximum consequences from a postulated scenario involving a series of system or component failures." (SNL/BNI)

MEAN RETURN PERIOD (MEAN RECURRENCE INTERVAL) - "The average time between events. For seismic events it means the average time between earthquakes or faulting events with specific characteristics (e.g., magnitude ≥ 6 in a specified region or in a specified fault zone." (Shah, et al., "Earthquake Spectra", Vol. 1, No. 1, 1984)

MESH - "The discrete network of points (nodes) approximately representing the continuous domain where the solution is sought. Used in conjunction with finite-difference and finite-element techniques." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

MITIGATION - "Means (1) avoiding the impact altogether by not taking a certain action or parts of an action; (2) minimizing impacts by limiting the degree or magnitude of the action and its implementation; (3) rectifying the impact by repairing, rehabilitating, or restoring the affected environment; (4) reducing or eliminating the impact over time by preservation and maintenance operations during the life of the action; or (5) compensating for the impact by replacing or providing substitute resources or environments." (10 CFR 960)

MODEL - "A conceptual or mathematical description of a physical system, subsystem, or component." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

NUMERICAL MODEL - "A mathematical representation of physical phenomena that requires the use of discrete numerical techniques for the solution of the governing equations. (Bear, J., "Dynamics of Fluid in Porous Media," 1972, Freeze, R., et al., "Groundwater", 1979).

COMMENTARY: As defined in 10 CFR 960, "Model" includes both conceptual and mathematical representations; this definition is considered too broad. Conceptual and mathematical models are defined subsequently. Mathematical models are further subdivided into analytical and numerical models. This classification is widely - if not universally - used.

PERCHED GROUND WATER - "Unconfined ground water separated from an underlying body of ground water by an unsaturated zone. Perched water conditions can occur when a relatively impervious layer of limited horizontal extent is located between the water table of an unconfined aquifer and the ground surface.: (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

PERFORMANCE ASSESSMENT - "An analysis that: (1) identifies the processes and events that might affect the disposal system; (2) examines the effects of these processes and events on the performance of the disposal system; and (3) estimates the cumulative releases of radionuclides, considering the associated uncertainties, caused by all significant processes and events. These estimates shall be incorporated into an overall probability distribution of cumulative release to the extent practicable." (40 CFR 191)

PERFORMANCE OBJECTIVE - "The predetermined standards or specifications used for the objective for evaluating each structure, system or component during the performance assessment.: (SNL/BNI)

PERMEABILITY - "A measure of the ability of subsurface materials to conduct fluids, characteristic of the medium alone." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

COMMENT: The term permeability is often used in lieu of hydraulic conductivity, although strictly speaking this convention is incorrect.

POROSITY: "The ratio of total void volume to total unit volume of a soil or rock, usually reported as a decimal fraction or a percentage." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

POSTCLOSURE EARTHQUAKE - "A reasonable earthquake ground motion for evaluating postclosure repository facilities. This ground motion is expected at the site with a return period of 10,000 years."

COMMENTARY: The definition is essentially that of SAND85-7104 (Blume, 1985). Comments similar to those for DE-1 and other SAND85-7104 design earthquakes apply.

PROBABILISTIC ANALYSIS - "A method to estimate the exceedance probability of a specified design event on the basis of a characterization of site region geologic structures and seismogenic sources, maximum magnitudes and recurrence statistics for each, and attenuation with distance of design event parameters. Uncertainties in these characterizations may be explicitly incorporated into the analysis."

COMMENTARY: This is a project-specific definition.

PROBABILISTIC SAFETY ASSESSMENT - "A method to estimate the exceedance probability of a specified scenario consequence. It incorporates the results of a probabilistic analysis of a specified design event with an assessment of the likely consequences of that event should it occur. Often, a number of scenarios leading to a particular consequence must be considered for an adequate safety assessment."

COMMENTARY: As proposed, this definition is a generalization to include the preclosure period of a performance assessment done in probabilistic terms. This is the heart of the repository licensing process.

REASONABLY FORESEEABLE EVENT - "An event that is reasonably likely to occur during the period of performance assessment and from which the design bases are derived." (10 CFR 60, SNL/BNI)

REASONABLE ASSURANCE - "The required confidence that the performance objectives will be met." (Fed. Reg. Vol. 48, 120, June 1983, 28204)

RESPONSE SPECTRUM - "A set of curves calculated from an earthquake accelerogram that gives values of peak response of a damped linear oscillator as a function of its period of vibration and damping."

COMMENTARY: This definition is taken verbatim from Shah, et al. (1984). It is very similar to Design Spectrum which should, perhaps, be shortened by reference to this definition.

RETARDATION FACTOR - "The ratio of the average ground-water velocity to the average radionuclide velocity. Retardation is the result of physical and chemical interactions between a radionuclide and the geohydrologic media through which it travels. The magnitude of the retardation factor is dependent upon the nature of the geologic materials, the fluid, and the chemical species."

COMMENTARY: We prefer to define the retardation factor rather than "radionuclide retardation," as is done in 10 CFR 960. The latter concept is ambiguous because it refers to both the process itself and its result.

RETRIEVABILITY - "The act of intentionally removing radioactive waste before repository closure from the underground location at which the waste had been previously emplaced for disposal." (10 CFR 960)

SATURATION (DEGREE OF) - "The ratio of the volume of fluids to the volume of voids in a unit volume of soil or rock." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

SATURATED ZONE - "That part of the subsurface located below the water table, wherein all pores are filled with water and fluid pressure is greater than atmospheric." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

SCENARIO - "A proposed sequence of events or conditions of which the resulting consequence is analyzed to determine related consequences." (SNL/BNI)

SEISMICITY - "The occurrence of earthquakes in space and time."

ALTERNATE DEFINITIONS: "The phenomenon of earth movements" ("Glossary of Geology", 1972). " (1) The likelihood of an area being subject to natural earthquakes, (2) The relative frequency, intensity or magnitude, and kind of natural earthquakes" ("Encyclopedic Dictionary of Exploration Geophysics", Sheriff, 1976).

COMMENTARY: The first definition is all that is needed although more elaborate definitions can be proposed (see above). The above definition is from Bolt ("Earthquakes, a Primer", 1978).

SEISMOGENIC PROVINCE - "A geologic area characterized by a similarity of geologic structure, tectonic setting, and earthquake characteristics. The province is a model of a seismic source for use in seismic design event analyses."

ALTERNATE DEFINITIONS: "A planar representation of a three-dimensional domain in the earth's lithosphere in which earthquakes are inferred to be of similar tectonic origin" (Shah, et al., 1984).

COMMENTARY: The first definition is paraphrased from one for "Tectonic Province" appearing in "Guidelines for Selecting Seismic Parameters for Dam Projects" (USCOLD, Draft, 1985). The concept is one of licensing significance as well as geotechnic input. It is a model, for licensing convenience, of a geologic region.

SENSITIVITY ANALYSIS - "A method whereby a problem is solved using a range of values of the input variables, in order to determine the relative influence of these variables upon the solution." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

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SITE - "An area contained within the boundary of a location under the effective control of persons possessing or using spent nuclear fuel or radioactive waste that are involved in any activity, operation, or process covered by this Subpart." (40 CFR 191)

SPECIFIC YIELD - "A measure of the storage capacity for an unconfined aquifer; it is defined as the volume of water that an unconfined aquifer releases from storage per unit surface area of the aquifer, per unit decline of the water table." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

SIGNIFICANT TECTONIC EVENT - "A tectonic design event."

COMMENTARY: As proposed here, this is just a special case of a design event. Note that it may be either anticipated or unanticipated and its significance is not really known until it has been considered in a performance assessment or probabilistic safety assessment.

STOCHASTIC - "Refers to the types of mathematical formulation wherein physical parameters, stresses, and/or boundary conditions are considered to be random variables with associated probability distributions." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

STORAGE COEFFICIENT - "A measure of the storage capacity for a confined aquifer; it is defined as the volume of water that a confined aquifer releases from surface, per unit surface area of the aquifer, per unit decline in hydraulic head." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

SUBSURFACE FACILITIES (UNDERGROUND) - "The underground structure and the rock required for support, including mined openings and backfill materials, but excluding shafts, boreholes, and their seals." (10 CFR 960)

SURFACE FACILITIES - "Repository support facilities within the restricted area." (10 CFR 60)

SURFACE WATER - "Any body of water located above ground surface, including fresh and salt water." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

TECTONIC PROCESSES - "A process contributing to the broad architecture of the outer part of the earth; that is, to the regional assembling of structural or deformational features and the study of their interrelationships, origins, and evolution through time."

COMMENTARY: This is modified version of 10 CFR 960.2 definition. Essentially unchanged. Not all tectonic processes are significant to repository licensing.

UNANTICIPATED EVENTS - "Those processes and events affecting the geologic setting that are judged not to be reasonably likely to occur during the period the intended performance objective must be achieved, but which are nevertheless sufficiently credible to warrant consideration. Unanticipated

processes and events may be either natural processes or events or processes and events initiated by human activities other than those activities licensed under this part. Processes and events initiated by human activities may only be found to be sufficiently credible to warrant consideration if it is assumed that: (1) The monuments provided for by this part are sufficiently permanent to serve their intended purpose; (2) the value to future generations of potential resources within the site can be assessed adequately under the applicable provisions of this part; (3) an understanding of the nature of radioactivity, and an appreciation of its hazards, have been retained in some functioning institutions; (4) institutions are able to assess risk and to take remedial action at a level of social organization and technological competence equivalent to, or superior to, that which was applied in initiating the processes or events concerned; and (5) relevant records are preserved, and remain accessible, for several hundred years after permanent closure. (10 CFR 60)

UNSATURATED ZONE - "That part of the subsurface located above the water table and above the capillary fringe, wherein pores are only partially filled with water and fluid pressure is less than atmospheric." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

COMMENT: 10 CFR 960 is unnecessarily restrictive by defining the unsaturated zone as the "zone between the land surface and the water table".

VALIDATION - "The process of checking a model through calibration (i.e., checking that the mathematical representation of the problem is consistent with the observed phenomena)." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

VERIFICATION - "The process of comparing the results obtained by a numerical model with an analytical solution of the same problem (i.e., verifying that the model does simulate the phenomena it is intended to represent)." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

VERY UNLIKELY EVENTS - "An event that is estimated to have between one chance in 100 and one chance in 10,000 of occurring within 10,000 years." (40 CFR 191)

VOLUMETRIC MOISTURE CONTENT - "The ratio of the volume of water in the pores to the total unit volume of soil or rock (when the total unit volume is the sum of the volumes of the solid portion, the water, and the air)." For saturated conditions, the moisture content equals the porosity. For unsaturated conditions, it is less than the porosity. (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

WATER TABLE - "The surface of a ground-water body at which the fluid pressure in the pores is atmospheric." (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

WETTING FRONT - The limiting surface of a body of infiltrating water which complete saturation can be assumed. (Bear, J., "Dynamics of Fluid in Porous Media", 1972, Freeze, R., et al., "Groundwater", 1979).

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V. J. Cassella, DOE/HQ (RW-22), FORSTL
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Terrence Bates, Weston, Rockville, MD
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JUL 11 1985

W. J. Purcell, Director, Office of Geologic Repositories, DOE/HQ (RW-20),
FORSTL

NNWSI PROJECT WEEKLY HIGHLIGHTS FOR WEEK ENDING JUNE 27, 1985

I. Issues Requiring Involvement of HQ or Other Projects

A. New Issues:

None to report.

B. Previously Reported Issues:

	<u>Issue</u>	<u>Status</u>	<u>First Report Date</u>
1.	Regarding March 19 letter to E. S. Burton - EA Briefings and Hearings - requested copy of documents generated as a result of "Roles and Responsibilities at Briefings" memo.	Open - Per ISGG Meeting 5/9-10, should be available 6/15.	5/14/85
2.	Regarding May 17 request for HQ to contact NRC for responses to NNWSI Project questions posed at the December DOE/NRC QA meeting.	Open	6/6/85
3.	Regarding June 6 request from Blanchard, when will Style Guides for EA and SCP be finalized? Need something in writing.	Open	6/20/85

II. Major Internal Concerns

None to report.

III. Significant Accomplishments (SA)/Information Items (II)

SA

Max Blanchard and Mike Foley met with Bob Loux on Friday, June 21 to clarify comments provided by the State on the EA. Barry Gale and Alan Benson also participated. Following the meeting, Barry and Alan discussed the newly created "desk" system for state interactions with Bob.

The Materials Review Board (MRB) reviewed the NNWSI Project's waste package studies at Livermore. There has been no contact between the MRB chairman and the Project Manager. This could be taken as a minor breach of etiquette.

II

Donald Vieth, along with various staff members, briefed the OCRWM Outreach Group (Chris Keilich et. al.) in Las Vegas on June 24 regarding the fact sheets and other educational information required to explain Yucca Mountain as a high-level radioactive waste repository. The group also toured the NTS on June 25 with Chris West (OPA).

Governor Bryan signed Senate Bill 56 on June 14, 1985. The bill creates a seven man commission to oversee the Nuclear Waste Policy Office. The new management structure is scheduled to be effective as of July 1. At this time it is not clear when the appointment of the seven-man commission will be complete. Names of people to serve have not yet been presented.

Donald Vieth was interviewed by Japanese television (Aomori Broadcasting Corporation) on Wednesday, June 26. They were interested in the experiments on dry storage conducted at E-MAD as well as the experiments conducted at Climax.

Donald Vieth made a presentation to the National Environmental Health Association entitled "Prospects of Yucca Mountain as a High Level Radioactive Waste repository". Approximately 20 people attended this session of the National meeting.

IV. Upcoming Events

1. Coordination Group Meetings

- o Monday-Tuesday, July 1-2: Institutional/Socioeconomic Coordination Group Meeting, Atlanta.

2. HQ Meetings

None to report.

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3. Internal Project and DOE/NV Meetings

- o Monday, July 1: SAIC Monthly Status Review.
- o Monday, July 1: SCP Management Group Meeting, Las Vegas.
- o Tuesday, July 9: SOC Meeting, NTS.
- o Tuesday, July 9: ESF Status Meeting, NTS.
- o Tuesday-Thursday, July 9-11: Waste Package QA Audit, Livermore.
- o Thursday-Friday, July 11-12: ESTP Committee Meeting, Denver.
- o Monday-Thursday, July 15-18: SCP Chapter 7 Internal Review, Las Vegas.
- o Monday-Wednesday, July 15-17: WMPO/USGS Meetings.
- o Thursday, July 18: Network Planning Review, SAIC, Las Vegas.
- o Monday, July 22: Tectonics Session, Las Vegas.
- o Wednesday-Thursday, July 24-25: PM-TPO Meeting, Las Vegas.


4. State and Public Interaction

- o Friday, June 28: Don Vieth to tour the Environmental Research Center at UNLV.
- o Wednesday, July 10: Pine County Commissioners/Ely Town Meeting.

5. NRC Interaction

- o Wednesday, July 3: Retrievability Position NRC Meeting - Generic (Tentative).
- o Thursday, July 18: Generic ES Meeting.
- o Tuesday-Wednesday, July 23-24: NRC/DOE Waste Package Meeting.

WMPO:DLV-1199


Donald L. Vieth, Director
Waste Management Project Office

JUL 22 1985

cc:

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R. J. Blaney, DOE/HQ (RW-22), FORSTL
C. R. Cooley, DOE/HQ (RW-24), FORSTL
M. W. Frei, DOE/HQ (RW-23), FORSTL
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JUL 22 1985

W. J. Purcell, Director, Office of Geologic Repositories, DOE/HQ (RW-20),
FORSTL

NNWSI PROJECT WEEKLY HIGHLIGHTS FOR WEEK ENDING JULY 18, 1985

I. Issues Requiring Involvement of HQ or Other Projects

A. New Issues:

None to report.

B. Previously Reported Issues:

Issue	Status	First Report Date
1. Regarding March 19 letter to E. S. Burton - EA Briefings and Hearings - requested copy of documents generated as a result of "Roles and Responsibilities at Briefings" memo.	Open - Per ISGG Meeting 5/9-10, should be available 6/15. Received Volume 1 of a seven-volume set on 6/28/85.	5/14/85

II. Major Internal Concerns

None to report.

III. Significant Accomplishments (SA)/Information Items (II)

SA

None to report.

II

A meeting that was scheduled on July 15-17 with WMPO and USGS was cancelled at the request of DOE/HQ. Don Vieth met with DOE/HQ to discuss the situation on July 16-18.

Internal review of SCP Chapter 7 was completed this week.

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Mitch Kunich gave a presentation on the Project to the Southern Nevada Homebuilder's Association on July 17 in Las Vegas. Approximately 60 people attended and were receptive to the presentation.

IV. Upcoming Events

1. Coordination Group Meetings

- o Tuesday-Wednesday, July 30-31: QACG Meeting.

2. HQ Meetings

- o Wednesday, August 6: Program Manager's Meeting, Denver

3. Internal Project and DOE/NV Meetings

- o Wednesday-Friday, July 17-19: Internal Review of SCP Chapter 3, Las Vegas.
- o Thursday, July 18: Network Planning Review, SAIC, Las Vegas.
- o Monday-Friday, July 22-26: Internal Review of SCP Chapter 3, continued, Las Vegas.
- o Monday-Tuesday, July 22-23: Internal Review of SCP Chapter 5, Las Vegas.
- o Monday, July 22: Tectonics Session, Las Vegas.
- o Monday-Thursday, July 22-25: WMPO QA Audit of WTSD, NTS.
- o Wednesday-Thursday, July 24-25: PM-TPO Meeting, Las Vegas.
- o Friday, July 26: SAIC Monthly Status Review, Las Vegas.
- o Monday, July 29: Computer QA SOP meeting, Las Vegas.
- o Tuesday, August 6: ESF Status meeting, NTS; SOC Meeting, NTS.

4. State and Public Interaction

- o Wednesday, July 25: Association of General Contractors' tour of NTS.
- o Monday, July 29: Texas Low-level Waste Disposal Authority, tour of NTS (Kunich).
- o Monday, August 5: Don Vieth to address Government and Business leaders of Portland, Oregon.

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- o Tuesday, August 6: Don Vieth to brief Tonopah City officials, Tonopah.
- o Thursday-Friday, August 8-9: First Repository States Meeting, Denver.

5. NRC Interaction

- o Friday, July 19: William Bland Presentation on QA, Las Vegas.
- o Tuesday-Wednesday, July 23-24: NRC/DOE Waste Package Meeting.
- o Wednesday, July 31: Retrievability Position NRC Meeting - Generic (Tentative).
- o Tuesday-Wednesday, August 20-21: Seismic/Tectonics NRC Meeting.
- o Tuesday-Wednesday, August 27-28: ESF Design NRC Meeting.
- o Tuesday-Wednesday, September 17-18: ESTP NRC Meeting.
- o Monday-Thursday, September 23-26: Hydrology/Geochemistry NRC Meeting.
- o Tuesday-Friday, October 1-4: Performance Assessment Plan NRC Meeting.

WMPO:DLV-1321


Donald L. Vieth, Director
Waste Management Project Office

JUL 18 1985

cc:

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M. W. Frei, DOE/HQ (RW-23), FORSTL
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JUL 18 1985

W. J. Purcell, Director, Office of Geologic Repositories, DOE/HQ (RW-20),
FORSTL

NNWSI PROJECT WEEKLY HIGHLIGHTS FOR WEEK ENDING JULY 11, 1985

I. Issues Requiring Involvement of HQ or Other Projects

A. New Issues:

None to report.

B. Previously Reported Issues:

Issue	Status	First Report Date
1. Regarding March 19 letter to E. S. Burton - EA Briefings and Hearings - requested copy of documents generated as a result of "Roles and Responsibilities at Briefings" memo.	Open - Per ISGG Meeting 5/9-10, should be available 6/15. Received Volume 1 of a seven-volume set on 6/28/85.	5/14/85
2. Regarding June 6 request from Blanchard, when will Style Guides for EA and SCP be finalized? Need something in writing.	Verbal commitment on 7/10 to a July 10 release.	6/20/85
3. The Generic Production Guide Manual that was to be issued by DOE/HQ on June 21 has not yet been received by the Projects.	Per HQ, is to be express mailed to Projects on July 10.	7/4/85

II. Major Internal Concerns

None to report.

III. Significant Accomplishments (SA)/Information Items (II)

SA

None to report.

II

Dennis Irby participated in a dry-run for the NRC ES generic meeting that is scheduled for July 18. The meeting was held in Denver.

Internal reviews for SCP Chapters 7 and 3 will be held in Las Vegas during the week of July 15-19. The Chapter 3 review will continue through the week of July 22-26.

The WMPO has selected a Systems and Project Control Branch Chief; Wendy Dixon will assume her duties near the end of July.

Don Vieth attended a Pine County Commissioners' meeting in Ely on July 10. The purpose of the meeting was to discuss a railway transportation route through the town of Ely. The commissioners presented their views to Don Vieth and he addressed their concern.

Don Hartman (MA-224.1) validated the FY 87 budget obligation authorization (BA) at \$15.3 million. A revised NNWSI request was submitted for \$19.7 million. The difference is associated with requirements to prefinance contractual activities associated with second shaft drilling and horizontal drift mining. Don Hartman's understanding is incomplete with regard to the need for added obligational authority. Second shaft drilling mobilization occurs in October 1987 which requires contract initiation in August or September 1987. Activities associated with underground breakout milestones M089 and M093 occur in FY 87. If these activities were performed by a subcontractor, full obligational authority associated with horizontal mining would be required in FY 87.

IV. Upcoming Events

1. Coordination Group Meetings

- o Tuesday-Wednesday, July 30-31: QACG Meeting.

2. HQ Meetings

- o Tuesday-Thursday, July 9-11: MRS Design Meeting at Bechtel, San Francisco.

JUL 18 1985

3. Internal Project and DOE/NV Meetings

- o Thursday-Friday, July 11-12: ESTP Committee Meeting, Denver.
- o Monday-Wednesday, July 15-17: WMPO/USGS Meetings.
- o Monday-Thursday, July 15-18: SCP Chapter 7 Internal Review, Las Vegas.
- o Wednesday-Friday, July 17-19: Internal Review of SCP Chapter 3, Las Vegas.
- o Thursday, July 18: Network Planning Review, SAIC, Las Vegas.
- o Monday-Friday, July 22-26: Internal Review of SCP Chapter 3, continued, Las Vegas.
- o Monday-Tuesday, July 22-23: Internal Review of SCP Chapter 5, Las Vegas.
- o Monday, July 22: Tectonics Session, Las Vegas.
- o Monday-Thursday, July 22-25: WMPO QA Audit of WTSD, NTS.
- o Wednesday-Thursday, July 24-25: PM-TPO Meeting, Las Vegas.
- o Thursday-Friday, July 25-26: Internal Review of SCP Chapter 8.4 and 8.7, Las Vegas.
- o Monday, July 29: Computer QA SOP meeting, Las Vegas.

4. State and Public Interaction

- o Thursday, July 25: Associated General Contractors of America (Southern Nevada Division of Nevada Chapter) tour of NTS (Kunich).
- o Monday, July 29: Texas Low-level Waste Disposal Authority, tour of NTS (Kunich).
- o Wednesday-Thursday, August 7-8: First Repository States Meeting, Denver.

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- o Monday-Thursday, September 23-26: Hydrology/Geochemistry NRC Meeting.
- o Tuesday-Friday, October 1-4: Performance Assessment Plan NRC Meeting.

WMPO:DLV-1284


Donald L. Vieth, Director
Waste Management Project Office

JUL 12 1985

cc w/encl:

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E. S. Burton, DOE/HQ (RW-25), FORSTL
J. J. Fiore, DOE/HQ (RW-22), FORSTL
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T. R. Clark, MGR
R. D. Duncan, DMGR
R. W. Taft, AMES
J. B. Cotter, EEM
D. H. Irby, EEM
M. B. Blanchard, WMPO, DOE/NV
M. P. Kunich, WMPO, DOE/NV
V. F. Witherill, WMPO, DOE/NV
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L. E. Perrin, RMB
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JUL 12 1985

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FORSTL**

NNWSI PROJECT MONTHLY REPORT FOR MAY 1985

**Enclosed is the NNWSI Monthly Report for May 1985 covering the technical
activities and status of the NNWSI Project.**

WMP0:DLV-1267

**Enclosure:
As stated**

Donald L. Vieth
**Donald L. Vieth, Director
Waste Management Project Office**