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B-0290

86/08/01/WK

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MEMORANDUM FOR: Ken Jackson, Section Leader
Geochemistry Section

FROM: John Bradbury
Walt Kelly
Paul Bembia
Geochemistry Section

SUBJECT: TRIP REPORT FOR VISIT TO ORNL, JULY 28-30, 1986

The main purpose of the visit to ORNL was to participate in a meeting on the use of EQ3/EQ6, the primary geochemical codes being used by the HLW projects in site characterization. An additional purpose was for the Division of Waste Management Director, Robert E. Browning, and WMGT Chief, Philip S. Justus, to meet ORNL staff members and tour laboratory facilities dedicated to our projects.

The meeting on EQ3/EQ6 was conducted by Dr. Teresa S. Bowers of MIT, an experienced user of the codes. An agenda is attached (attachment #1). The participants are listed in attachment #2.

On the first day, Dr. Bowers presented some of her work on oceanic hot springs chemistry which included an application of EQ3/EQ6. Following this opening presentation, she led a discussion on EQ3, the thermodynamic speciation code. Dr. Bowers pointed out the strengths and weaknesses of the EQ3 code and highlighted potential problem areas. Of greatest concern is the quality of the thermodynamic data base, especially at high temperatures and ionic strengths. Data for iron and aluminum oxides and chloride species are especially weak. The statement was made that the code has outstripped the database.

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A discussion of EQ6, the mass transfer code, was held the second day. Walt Kelly attempted to run the code with some data collected at Sheffield; however, we were unable to complete the exercise in the time alotted.

The codes have impressive capabilities and a number of new capabilities are being added or planned. Presently, the codes can model geochemical scenarios involving liquids at high ionic strength, high temperature, variable pressure and solids having variable compositions. The new capabilities may include ion exchange, sorption, diffusion, and kinetics. The quality of the data base is the critical parameter in the usefulness of model results, however, and the NRC should stress to DOE the primacy of research for its improvement. The codes, especially EQ6, are very complicated. For the NRC staff to use the codes on a part-time basis, some instruction would be necessary. Dr. Bowers, who uses the codes routinely, says that she commonly encounters bugs, and updates to the codes are frequent. Also, there is no formal documentation for EQ6 yet. At this time, our contractors at ORNL are in a better position to use the codes. Once ORNL has the codes in proper running order, NRC staff may be in a better position to apply them. (NRC has an account on the ORNL computing facilities.)

During the two days, we also had an opportunity to tour ORNL LLW disposal facilities and geochemical laboratories. Steve Stow gave us a tour of some of the LLW disposal facilities, including the hydrofracturing disposal facility which was closed two years ago due to detection of radionuclide migration. He also showed us a field experiment designed to gather data on trace metal migration in soils.

On Tuesday afternoon, we toured some laboratories used by the Chemical Division for characterizing hydrothermal solutions. We were shown large volume rocking autoclaves which could maintain temperatures to a few hundreths of a degree at

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temperatures less than 500°C and pressures less than 2 kilobars. These bombs were used in experiments to study the solubility of magnetite in acetate solutions. These experiments employed the same techniques used to determine the solubility of radionuclide-bearing solid phases at elevated temperatures.

A novel technique will be employed to determine the pressure-volume-temperature relations of hydrothermal solutions (e.g. CO_2-H_2O). Densities of the solutions will be determined by comparing the vibrational frequency of a "tuning fork" containing an unknown solution relative to the frequency containing a solution of known density. This technique should produce densities accurate to three decimal places. The results of these experiments can be used for determining the thermodynamic properties of hydrothermal solutions similar to the ones that will pass through the repository.

We saw another experiment in which the pH of solutions were being determined at temperatures up to 300°C under reducing conditions. This tour left us with the impression that, contrary to popular belief, chemical reactions of geologic materials can be characterized with high precision at elevated temperatures. In fact, kinetics of reactions at higher temperatures pose less of a problem for the experimentalist because equilibrium is approached more quickly. Futhermore, the number of species dissolved in aqueous solutions at high temperatures decreases due to the decrease in the dielectric constant for H_2O.

On Wednesday, 1986 R.E. Browning, P.S. Justus, and J.W. Bradbury met with the NRC contractors working on B0290, "Laboratory Evaluation of DOE Radionuclide Solubility Data and Selected Retardation Parameters, Experimental Strategies, Laboratory Techniques, and Procedures" and B0287 "Technical Assistance in Geochemistry". Attached are a schedule and a list of attendees of the meeting (Attachments #3 and #4).

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G.K. Jacobs gave a presentation on the NRC nuclear waste programs at ORNL. Attached is the package of viewgraphs discussed in the talk (Attachment #5). Most of the discussion between NRC representatives and the Oak Ridge contractors centered around three major topics:

1) Effect of NRC geochemistry contracts on DOE's program
2) QA programs at Oak Ridge
3) Effect of FFRDC on B0290 and B0287

The question arose concerning the impact of the NRC geochemistry contracts on the DOE program. Is the DOE listening to suggestions from the NRC geochemists and geochemical contractors and is the DOE evaluating and, if necessary, changing their program accordingly? The use of hydrazine in sorption experiments to control Eh was given as an example. Several years ago the contractors on B0290 showed that hydrazine may produce reactions not expected in a HLW repository. This would make the results from these experiments suspect when applied to a repository. The DOE has responded to reports from Oak Ridge describing the uncertainties associated with experiments using hydrazine. They acknowledge the potential problems of hydrazine but continue to study the possibility that some parts of the hydrazine experiments may be useful for characterizing the HLW sites.

The hydrazine problem illustrates that resolution of a single experimental geochemistry issue can take several years. Contributing to the length of time for resolution of geochemical issues is the duration of experiments, the time it takes to analyze and publish the results, and the time it takes for the counter experimentation, analysis, and publication. Informal visits (Appendix 7) to the DOE contractor laboratories to discuss methodologies might accelerate the issue resolution process.

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It was noted in the meeting that the impact of the Oak Ridge work on the DOE program may be greater than first perceived. For example, at the Appendix 7 visit at Los Alamos last fall, the NRC and their contractors listed a number of concerns about sorption experimentation. The DOE contractors responded at that time by saying that they have investigated or are currently investigating every concern listed. One concern was that little sorption work has been done on the actinides. Los Alamos has published voluminous quantities of information on the simple cations, Sr, Cs, and Ba, but has published little on the actinides. The reason given for the lack of published information on the actinides is that the experimental results are indecipherable. Since Oak Ridge focuses on problem areas in solubility and sorption determinations, and DOE and their contractors do not publish data they do not understand, the tendency is to see little apparent impact on the DOE experimental program. Appendix 7 visits and/or Data Reviews, however, do disclose that program directions have changed in response to our contractor work.

The Quality Assurance program(s) at Oak Ridge were described by G.K. Jacobs. Oak Ridge has a laboratory-wide QA program and other QA programs for the individual divisions of the laboratory. The Quality Assurance programs are based on the concept that good scientific methodology assures quality of the results.

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The contractors were concerned about the future of the contracts in light of the FFRDC. They were told that, pending a drastic turn-of-events, both contracts would be funded for one more year at a level approximating that for FY86.

John W. Bradbury

Walton R. Kelly

Paul J. Bembia

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July 22, 1986

The schedule for Teresa Bowers visit is as follows:

Monday July 28	9:30 a.m. Seminar entitled "Chemical and isotopic systematics of oceanic hot springs." Building 1505, room 344.
	10:30-12:30 p.m. Time for individual discussions.
	12:30-1:30 p.m. Lunch - cafeteria.
	1:30-4:30 p.m. EQ3NR presentation and discussion. Building 1505, room 344.
	Dinner - probably "Big Ed's" for pizza.
Tuesday July 29	9:00 a.m. EQ6 presentation and discussion. Building 1505, room 344.
	1:00 p.m. Continuation of EQ6 questions or time for individual discussions with T. Bowers. Building 1505, room 344 is reserved.

Please let me know if you would like to meet with Dr. Bowers individually or join us for dinner.

You should have received a copy of the EQ3NR manual. Please bring it and any questions you may have on the use of these programs with you.

Karen

Karen Von Damm
(6-0427)

Attachment #2

86/08/14

List of Attendees
EQ3/6 Workshop at Oak Ridge
July 27-28, 1986

W.D. Arnold
R.W. Arnseth
P.J. Bembia, WMGT
J.G. Blencoe
T.S. Bowers
J.W. Bradbury, WMGT
D.R. Cole
G.K. Jacobs
W.R. Kelly, WMGT
A.D. Kelmers
L.A. Kovach, RES
G.D. O'Kelley
S.H. Stowe
K.L. VonDamm

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Oak Ridge National Laboratory
Trip Schedule
for R. Browning and P. Justus
July 30, 1986

11:00	Arrive Knoxville
11:45	Arrive Oak Ridge National Laboratory
12:00	Lunch with contractors
1:00	Program Overview
1:45	Discussion on contracts - Gary Jacobs
	B0290 * - Laboratory Evaluation of DOE Radionuclide Solubility Data and Selected Retardation Parameters, Experimental Strategies, Laboratory Techniques, and Procedures
	B0287 * - Technical Assistance in Geochemistry
2:30	Tour of Laboratory - Bob Meyer
3:15	Meeting with A.P. Malinauskas
3:45	Leave for Knoxville

* see attached Project Descriptive Summaries

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Attachment #4

86/08/08/JWB

List of Attendees
Meeting with NRC Contractors at Oak Ridge
July 30, 1986

R.E. Browning, Director, DWM
P.S. Justus, Acting Branch Chief, WMGT
J.W. Bradbury, WMGT
G.K. Jacobs
J.G. Blencoe
R.M. Gove
A.D. Kelmers
R.E. Meyer
G.D. O'Kelley
K.L. VonDamm
V.S. Tripathi
W.D. Arnold

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ORNL WSC-48066

REVIEW OF NRC WASTE PROGRAMS

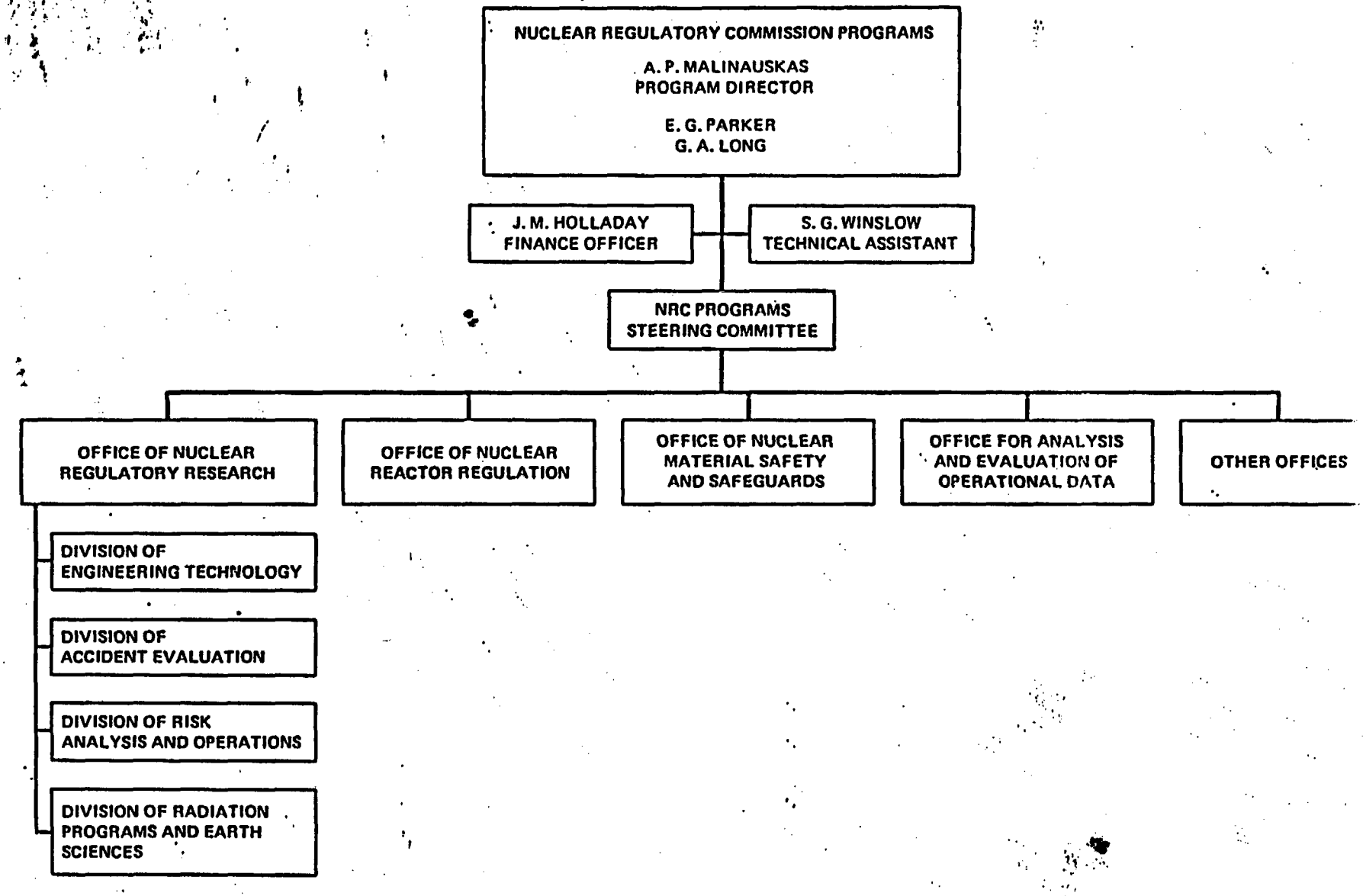
Gary K. Jacobs

Environmental Sciences Division

July 30, 1986

Oak Ridge National Laboratory

Attachment #5


NUCLEAR REGULATORY COMMISSION PROGRAMS
A. P. MALINAUSKAS
PROGRAM DIRECTOR
E. G. PARKER
G. A. LONG
J. M. HOLLADAY
FINANCE OFFICER
S. G. WINSLOW
TECHNICAL ASSISTANT
NRC PROGRAMS
STEERING COMMITTEE
OFFICE OF NUCLEAR
REGULATORY RESEARCH
OFFICE OF NUCLEAR
REACTOR REGULATION
OFFICE OF NUCLEAR
MATERIAL SAFETY
AND SAFEGUARDS
OFFICE FOR ANALYSIS
AND EVALUATION OF
OPERATIONAL DATA
OTHER OFFICES
DIVISION OF
ENGINEERING TECHNOLOGY
DIVISION OF
ACCIDENT EVALUATION
DIVISION OF RISK
ANALYSIS AND OPERATIONS
DIVISION OF RADIATION
PROGRAMS AND EARTH
SCIENCES

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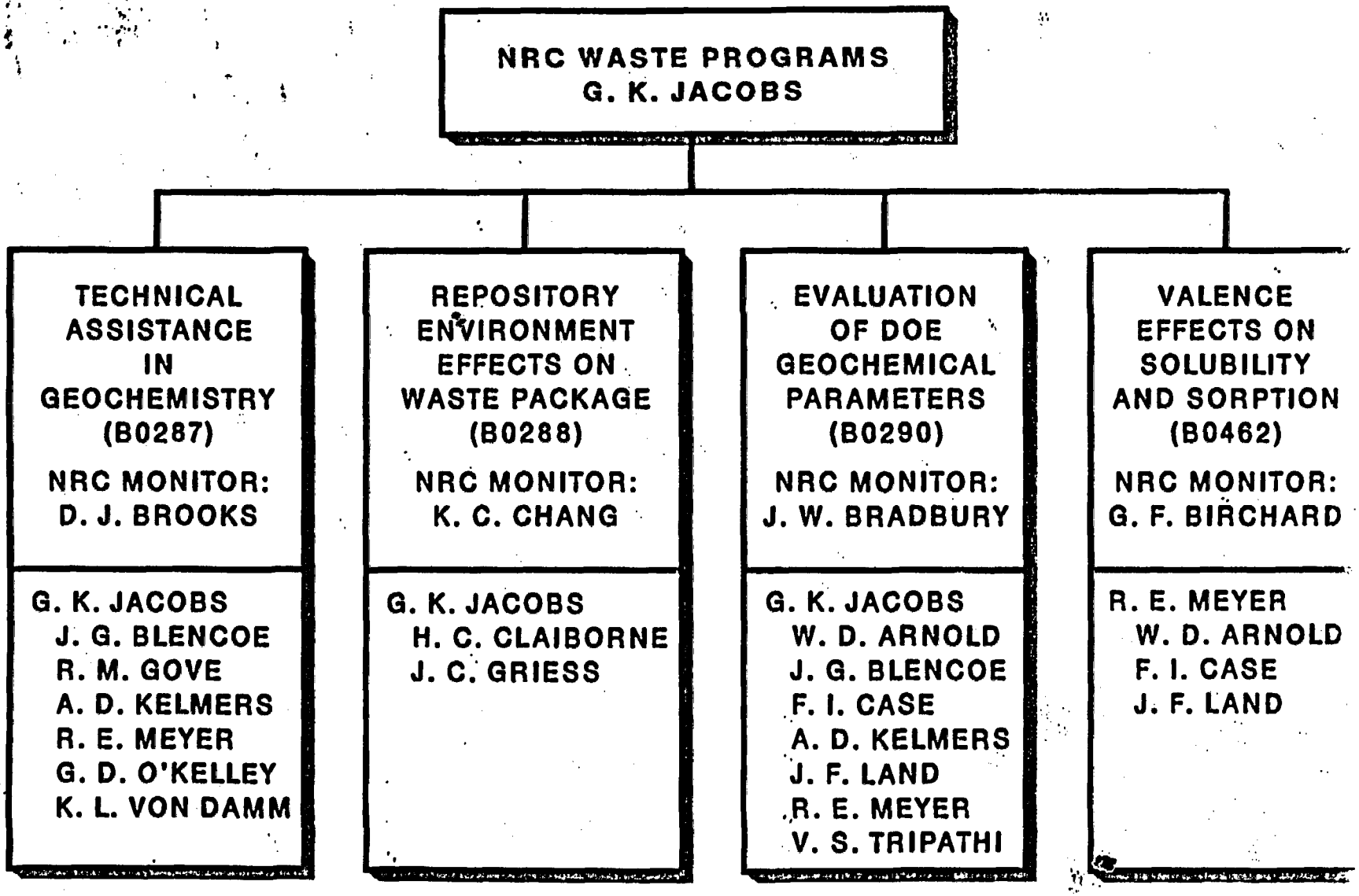

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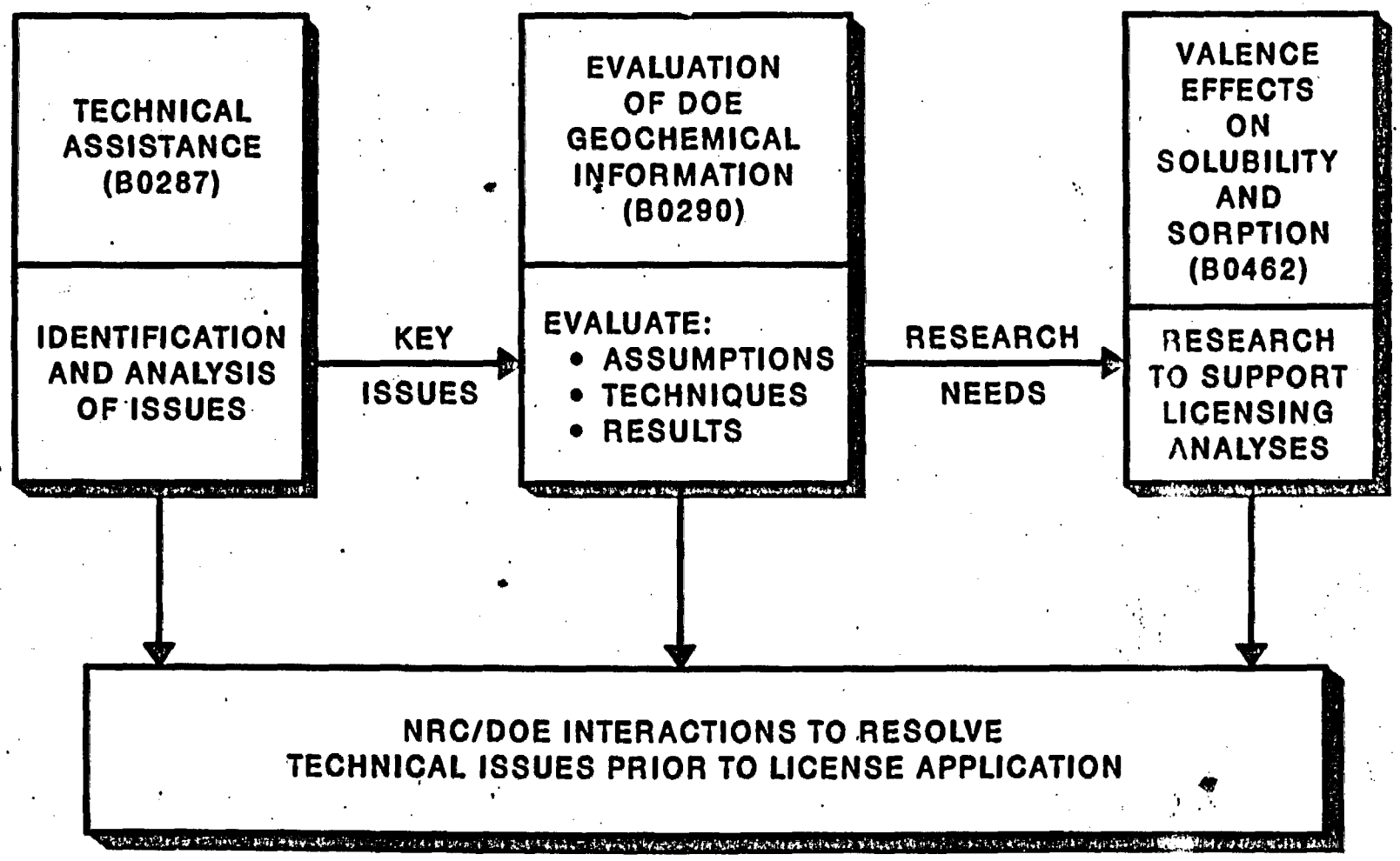
RELATIONSHIP AMONG GEOCHEMISTRY PROJECTS



GEOCHEMICAL ASPECTS OF HLW ISOLATION

- GEOCHEMICAL CONDITIONS
- WASTE/BARRIER/ROCK/WATER INTERACTIONS
- SOLUBILITY
- SORPTION

EXAMPLE OF PROJECT INTERACTIONS

B0287

- REVIEW AND ASSESSMENT OF SORPTION INFORMATION FOR HANFORD SITE
- IDENTIFIED ISSUE OF REDOX CONTROL DURING EXPERIMENTATION

B0290

- EVALUATION OF SORPTION ONTO BASALT
- INCLUDED STUDY OF REDOX CONTROL
- IDENTIFIED NEED FOR ADDITIONAL INFORMATION ON TECHNETIUM

B0462

- DETAILED INVESTIGATION OF VALENCE EFFECTS ON TECHNETIUM SOLUBILITY AND SORPTION

- *IDENTIFICATION OF KEY INFORMATION NEEDED FOR DOE TO RESOLVE ISSUE OF TECHNETIUM SORPTION*

TECHNICAL ASSISTANCE IN GEOCHEMISTRY (B0287)

OBJECTIVE:

TO SUPPORT NRC STAFF ANALYSIS OF DOE'S GEOCHEMICAL INFORMATION

- COLLECT AND REVIEW DATA AND REPORTS
- PARTICIPATE IN NRC/DOE WORKSHOPS
- TECHNICAL REPORTS ON KEY ISSUES
- REVIEW MAJOR PLANNING DOCUMENTS OF DOE
- SHORT-TERM TECHNICAL ASSISTANCE

TECHNICAL ASSISTANCE IN GEOCHEMISTRY (B0287)

HIGHLIGHTS (FY 1986)

- REVIEW OF ENVIRONMENTAL ASSESSMENTS
- WORKSHOP ON SORPTION
- LETTER REPORTS (40 THROUGH JULY 1986)
- WASTE MANAGEMENT DOCUMENT DATA BASE
- TOPICAL REPORTS
  - MATRIX DIFFUSION
  - SOLUBILITY INFORMATION FOR THE HANFORD SITE

TECHNICAL ASSISTANCE IN GEOCHEMISTRY (B0287)

SORPTION WORKSHOP:

- SORPTION CAN BE AN IMPORTANT COMPONENT OF REPOSITORY PERFORMANCE
- UNDERSTANDING OF SORPTION PROCESSES WILL BE NECESSARY FOR SOME RELEASE SCENARIOS
- UNDERSTANDING MUST BE DEVELOPED THROUGH LABORATORY INVESTIGATIONS COMPLEMENTED BY FIELD AND NATURAL ANALOG STUDIES
- IMPORTANT PARAMETERS FOR STUDY WERE IDENTIFIED AND DISCUSSED

EVALUATION OF DOE GEOCHEMICAL INFORMATION (B0290)

OBJECTIVE:

TO INDEPENDENTLY EVALUATE DOE'S INFORMATION ON SOLUBILITY, SORPTION, AND GEOCHEMICAL CONDITIONS

- METHODS, ASSUMPTIONS, AND RESULTS
- UNCERTAINTY, ACCURACY, AND CONSERVATISM

EVALUATION OF DOE GEOCHEMICAL INFORMATION (B0290)

HIGHLIGHTS (FY 1986)

- COMPLETED EVALUATION OF HANFORD SITE
  - HYDRAZINE INAPPROPRIATE
  - Tc SORPTION ON BASALT NOT EFFECTIVELY DEMONSTRATED BY DOE
  - SIGNIFICANT SORPTION OF NP UNDER ANOXIC CONDITIONS
  - FORMATION OF Na-BOLTWOODITE COMPLICATES SORPTION OF URANIUM

ORNL WS-48074

EVALUATION OF DOE GEOCHEMICAL PARAMETERS (B0290)

HIGHLIGHTS (FY 1986)

- STARTED EVALUATION OF YUCCA MOUNTAIN
  - PREPARATION OF MATERIALS
  - DEVELOPMENT OF METHODS
  - EARLY RESULTS WITH Cs, Sr, Eu, Np
  - COMPLEX MINERALOGY AND HYDROLOGY

EVALUATION OF DOE GEOCHEMICAL INFORMATION (B0290)

HIGHLIGHTS (FY 1986)

- EVALUATION OF Kd AND RETARDATION FACTOR PARAMETERS FOR ADEQUACY IN MODELING RADIONUCLIDE SORPTION
  - COMPREHENSIVE MODELING WITH A FULL-FEATURED GEOCHEMICAL MODEL COUPLED TO A HYDROLOGIC TRANSPORT MODEL
  - RESULTS TO BE PRESENTED DURING SYMPOSIUM AT AMERICAN CHEMICAL SOCIETY NATIONAL MEETING

PLANNED ACTIVITIES

B0287

- REVIEW OF SITE CHARACTERIZATION PLANS
- WASTE MANAGEMENT DOCUMENT DATA BASE
- LETTER REPORTS
- WORKSHOPS
- ANALYSIS OF ISSUES

PLANNED ACTIVITIES

B0290

- EVALUATION OF YUCCA MOUNTAIN INFORMATION
  - METHODS
  - IDENTIFICATION OF KEY MINERALS FOR SORPTION
  - KEY NUCLIDES (Np, U, Pu, Am)
  - GEOCHEMICAL CONDITIONS FOR WASTE PACKAGE
  - COLLOIDS
  - COLUMN METHODS

PLANNED ACTIVITIES

B0462

- SOLUBILITY/SORPTION IN BRINES