See Porket 2 for end. 48 ر تو حصو τ. UNITED STATES NUCLEAR REGULATORY COMMISSION

WASHINGTON, D.C. 20555

February 12, 1985

Linda,

I am sending this along to you--thought you would be interested.

WM Record File	WM Project Docket No		
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Los Alamos

NNWSI

# **PROJECT** Geochemistry Presentation to January TPO Meeting

8502270352	850131	
PDR WASTE	PDR	



#### Los Alamos

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# OVERVIEW

# G. L. DEPOORTER



LOS ALAMOS LABORATORY CONTRIBUTION TO SITE AND REPOSITORY INVESTIGATIONS

Los Alamos

## WBS 2.3.4.1 GEOCHEMISTRY

## WBS 2.3.4.2 MINERALOGY/PETROLOGY

## WBS 2.4.2.3.2 SEALING MATERIALS EVALUATION



# S GEOCHEMISTRY TESTS IN Los Alamos EXPLORATORY SHAFT

**CHLORINE-36 TEST** 

COLLECT SAMPLES FROM THE EXPLORATORY SHAFT AS IT IS MINED AND USE COSMOGENIC <sup>36</sup>CI AS A TRACER TO DETERMINE THE VELOCITY OF WATER MOVEMENT THROUGH THE UNSATURATED ZONE

#### APPLIED DIFFUSION

DETERMINE WHETHER THE RESULTS OF LABORATORY-SCALE DIFFUSION MEASUREMENTS CAN BE EXTRAPO-LATED ACCURATELY TO PREDICT THE RATES OF AQUEOUS TRANSPORT OF NONSORBING RADIOACTIVE WASTE SPECIES



- GROUNDWATER CHEMISTRY (A. E. OGARD)
- NATURAL ISOTOPE CHEMISTRY (A. E. NORRIS)
- HYDROTHERMAL GEOCHEMISTRY (C. J. DUFFY)
- SOLUBILITY DETERMINATION (J. F. KERRISK)
- SORPTION AND PRECIPITATION (K. W. THOMAS)
- DYNAMIC TRANSPORT PROCESS (R. S. RUNDBERG)
- RETARDATION SENSITIVITY ANALYSIS (B. J. TRAVIS)



- ALTERATION MINERALOGY
- MINERAL STABILITY
- MINERALOGY OF TRANSPORT PATHWAYS
- EXPLORATORY SHAFT MINERALOGY/ PETROLOGY



- 10 CFR 60
- REGULATORY GUIDE 4.17
- NRC DRAFT TECHNICAL POSITION ON RADIONUCLIDE SOLUBILITY IN GROUNDWATER
- CLOSEOUT COMMENTS FROM JANUARY 1983
  GEOCHEMISTRY WORKSHOP
- CLOSEOUT COMMENTS FROM JULY 1984
  GEOCHEMISTRY WORKSHOP

## KEY ISSUES FROM ORANGE Los Al DRAFT SCR

2230H

TASK	MIRERALOGI	N // GROUNDWATER I // CHEMISTRY CH	ATURAL SOTOPE EMISTRY	HYDROTHERMAL GEOCHEMISTRY	SOLUBILITY	SORPTION/ PRECIPITATION	DYNAMIC TRANSPORT	RETARDATION SENSITIVITY	APPLIED DIFFUSION	SEAL MATERIA EVALUATI
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#### CORRELATION OF LANL Los Alamos WORK WITH NRC ISSUES FROM ISTP FOR NNWSI



Los Alamos

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# AND PETROLOGY VANIMAN WBS 2.3.4.2 MINERALOGY **\_**

# Los Alamos **MINERALOGY-PETROLOGY: ISSUE 1.2**

LOGIC PATHS, FLUXES, VELOCITIES, AND TRAVEL TIMES"

ATION NEEDS:

- CONSTRAINTS ON DEPTH AND EXTENT OF EMPLACE-MENT HORIZON ?
  - **DEFINITION OF ACCESSIBLE ENVIRONMENT?**
- WHAT ARE THE UNSATURATED FLOW PATHS?
- WHAT ARE THE SATURATED FLOW PATHS?
- **EFFECTS OF THERMAL PULSE ON ROCK PROPERTIES**, **PERMEABILITY, SATURATION ?**



"WHAT DEGREE OF RADIONUCLIDE RETARDATION WILL BE ATTAINED ?"

INFORMATION NEEDS: 1 1913 Contraction of the Party of the

- 1.3.1 SORPTION PROCESSES?
- 1.3.2 PRECIPITATION PROCESSES?
- 1.3.4 BOUNDS ON OVERALL RETARDATION ?

## MINERALOGY-PETROLOGY: Los Alamos ISSUE 3.3

#### "IMPACTS ON COST OR SAFETY"

22301

INFORMATION NEEDS:

• 3.3.1 - TARGET HORIZON CONTINUITY ?



"COST-EFFECTIVE FOR TRANSPORT, EMPLACEMENT, AND POSSIBLE RETRIEVAL"

**INFORMATION NEEDS:** 

- 3.4.1 BOUNDARIES OF THE REPOSITORY BLOCK?
- 3.4.2 ALLOWABLE GROSS THERMAL LOADING ?

#### **ISSUES/TASKS MATRIX FOR** Los Alamos **MINERALOGY-PETROLOGY**





#### MINERALOGY-PETROLOGY Los Alamos STUDIES ARE SUBDIVIDED INTO FOUR ELEMENTS

- ALTERATION MINERALOGY
- MINERAL STABILITY
- MINERALOGY OF TRANSPORT PATH-WAYS
- EXPLORATORY SHAFT MINERALOGY AND PETROLOGY



# FRACTURE MINERALOGY – PAST FLOW PATHS, FLOW TIMES, AND TRANSPORT PHENOMENA

# NATURAL ALTERATION -

TIMING, TEMPERATURES, AND TECTONIC RELATIONS OF PAST ALTERATION



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 GEOLOGIC RECORD OF HYDROTHERMAL ALTERATION AT YUCCA MOUNTAIN

- DEHYDRATION KINETICS IN SMECTITES, ZEOLITES, AND GLASSES
- CATION-EXCHANGE CAPABILITIES OF ZEOLITES AFTER PROLONGED HEATING

 EXPERIMENTS ON LOW—TEMPERATURE ALTERATION, TOPOPAH SPRING VITROPHYRE (LLNL)





- HYDRATION CAPABILITY IS COUPLED TO SORPTION CAPABILITY. WILL ZEOLITES REHYDRATE AFTER 100–1000 YEARS AT 100°C ?
- WILL THE CATION EXCHANGE CAPACITY OF ZEOLITES BE AFFECTED AFTER 100–1000 YEARS AT 50–100°C ?
- WILL GLASS ALTERATION BE SIGNIFICANT ?
  (TOPOPAH VITROPHYRE EXPERIMENTS WITH LLNL)

# NNERALOGY OF Los Alamos TRANSPORT PATHWAYS

- HOST ROCK PETROGRAPHY; MEASURES OF CONTINUITY AND OF VARIABILITY
- THREE DIMENSIONAL MINERALOGIC MODEL OF YUCCA MOUNTAIN
- LIMITS ON DISTRIBUTION AND ABUNDANCE OF FERROUS IRON
- QUANTITATIVE X-RAY DIFFRACTION ANALYSIS
- STATISTICAL EVALUATION OF THREE-DIMENSIONAL MINERALOGIC MODELS



DEPTH

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Major Clinoptilolite/Mordenite Intervals

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Major Clinoptilolite/Mordenite Intervals H-5 below 760 m from Beatly, et al. central part of H-6 from Craig, et al.

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- IMPROVEMENTS ON AND TESTS OF TOPOPAH SPRING INTERNAL PETROLOGY: REALISTIC MINING ENVIRONMENT
- CRITICAL PETROLOGIC TRANSITIONS UNDERLYING THE DEVITRIFIED TOPOPAH SPRING MEMBER: ZEOLITE/CLAY, VITROPHYRE, VITRIC NONWELDED, ZEOLITE
- FRACTURE MINERALOGY IN LARGE SAMPLES: SPOILS OF MINING
- MAPPING SUPPORT (USGS)

#### GENERALIZED LITHOLOGY OF TOPOPAH SPRING VITROPHYRE

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#### TIMETABLE FOR MINERALOGY-PETROLOGY COMPLETIONS

Los Alamos

- ALTERATION MINERALOGY 6/86
  MINERAL STABILITY 12/86
- MINERALOGY OF TRANSPORT PATHWAYS 6/89\*
- EXPLORATORY SHAFT MINERALOGY AND PETROLOGY 3/89\* \*DEPENDENT ON ES SCHEDULE

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--- Los Alamos

# HYDROTHERMAL GEOCHEMISTRY WBS 2.3.4.1.3 C. J. DUFFY



- PRODUCE A CONCEPTUAL MODEL FOR THE EVOLUTION OF YUCCA MOUNTAIN TO ITS PRESENT MINERALOGIC STATE
- PREDICT THE FUTURE STATES OF YUCCA MOUNTAIN FOR TIMES IMPORTANT FOR A REPOSITORY

## -INCLUDES

- NATURAL CHANGES
- CHANGES DUE TO REPOSITORY EMPLACEMENT





#### ISSUES

- 1.1.1 ESTIMATES OF AND BOUNDS ON THE FLOW OF STEAM, AIR, AND WATER IN THE WASTE PACK-AGE EMPLACEMENT ENVIRONMENT
- 1.1.2 ESTIMATES OF AND BOUNDS ON THE CHEMICAL CHARACTERISTICS OF STEAM, AIR, AND WATER, IN THE HORIZON AND WASTE PACKAGES
- 1.2.1 ESTIMATES OF BOUNDS ON THE GEOLOGIC FRAMEWORK OF THE SITE, INCLUDING THE LOCATIONS OF ANY STRATIGRAPHIC OR STRUCTURAL CONSTRAINTS ON THE DEPTH AND LATERAL EXTENT OF THE WASTE-EMPLACEMENT HORIZON
- 1.2.3 ESTIMATES OF AND BOUNDS ON HYDROLOGIC FLOW PATHS, FLUXES, WATER VELOCITIES, AND TRAVEL TIMES IN THE UNSATURATED ZONE
- 1 2.5 ESTIMATES OF AND BOUNDS ON THE EFFECTS OF THE REPOSITORY-INDUCED THERMAL PULSE AND ROCK EXCAVATIONS ON ROCK-MASS PROPERTIES AND THE RESULTING EFFECTS ON THE PERMEABILITY AND DEGREE OF SATURATION IN THE UNSATURATED AND SATURATED ZONES
- **1.3.1 ESTIMATES OF AND BOUNDS ON RADIONUCLIDE RETARDATION BY SORPTION PROCESSES**
- **1.3.2 ESTIMATES OF AND BOUNDS ON RETARDATION BY PRECIPITATION PROCESSES**
- 1.3.4 CALCULATED ESTIMATES OF AND BOUNDS ON RADIONUCLIDE RETARDATION ALONG THE HYDROLOGIC FLOW PATHS WITHIN THE REPOSITORY AND BETWEEN THE REPOSITORY AND THE ACCESSIBLE ENVIRONMENT
- 1.4.1 DEFINITION OF BOUNDARIES OF THE WASTE PACKAGE, ENGINEERED BARRIER SYSTEM, DISTURBED ZONE, AND ACCESSIBLE ENVIRONMENT
- 1.4.2 CALCULATED ESTIMATES OF AND BOUNDS ON THE PERFORMANCE OF THE TOTAL WASTE ISOLATION SYSTEM, INCLUDING WASTE PACKAGE RELEASE RATES, GROUNDWATER TRAVEL TIME, RETARDATION OF RADIONUCLIDES, AND THE INTEGRATED RELEASE OF RADIO-NUCLIDES TO THE ACCESSIBLE ENVIRONMENT A FUNCTION OF TIME
- 2.2.5 CALCULATED ESTIMATES OF AND BOUNDS ON THE RATES AND CONCENTRATIONS OF RADIO-NUCLIDE RELEASES FROM THE REPOSITORY TO THE ACCESSIBLE ENVIRONMENT RESULTING FROM FUTURE CLIMATIC CONDITIONS AND TECTONISM



## TYPES OF DATA TO BE OBTAINED

- THERMODYNAMIC DATA FOR ZEOLITE SOLID SOLUTIONS
- THERMODYNAMIC DATA FOR CLAY SOLID SOLUTIONS
- DATA ON THE EFFECTS OF AI/Si ORDERING ON THE THERMODYNAMICS OF ALKALI FELDSPARS
- KINETIC DATA ON MINERAL DISSOLUTION AND PRECIPITATION
- MINERALOGIC AND WATER COMPOSITION DATA FROM HOT SPRING DEPOSITS IN TUFF



- KINETIC DISSOLUTION/PRECIPITATION MODELS
- COUPLED MASS TRANSPORT AND KINETIC
  MODELS
## WHAT CAN BE Los Alamos CALCULATED?

EQ3/6

- EQUILIBRIUM MINERAL ASSEMBLAGES AND WATER COMPOSITIONS
- FUTURE VERSIONS MAY CONTAIN KINETICS

**KINETIC DISSOLUTION/PRECIPITATION MODELS** 

• RATE OF CHANGE OF METASTABLE MINERAL ASSEMBLAGES AND WATER COMPOSITIONS

**COUPLED MASS TRANSPORT AND KINETIC MODELS** 

- DISTRIBUTION OF METASTABLE MINERAL ASSEMBLAGES AND FLUID COMPOSITIONS
- RELATIONSHIP OF FLUID FLUX TO METASTABLE MINERAL DISTRIBUTION



• DO THEY EXPLAIN OBSERVATION IN YUCCA MOUNTAIN ?

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- DO THEY EXPLAIN OBSERVATIONS IN HOT SPRING DEPOSITS IN TUFF ?
- DO THEY EXPLAIN LITERATURE DATA ON ALTER-ATION OF VITRIC TUFFS ?

#### S S PROJECT ESTIMATES OF AND Los Alamos BOUNDS ON RADIONUCLIDE RETARDATION

# BY SORPTION PROCESSESDEPENDENT ON MINERALOGY

# BY PRECIPITATION PROCESSES

 DEPENDENT ON WATER CHEMISTRY
 DEPENDENT ON MINERALS THAT MAY BE PRECIPITATING



- WATER MOVEMENT THROUGH THE UNSATURATED ZONE, COUPLED WITH MINERAL AND GLASS DISSOLUTION AND PRECIPITATION RATES, DETERMINES THE DISTRIBUTION OF MINERALS
- MODELING THE DEVELOPMENT OF THE PRESENT MINERAL DISTRIBUTION CAN PROVIDE ESTIMATES OF THE FLOW PATHS, FLUXES, WATER VELOCITIES, AND TRAVEL TIMES



- CLINOPTILOLITE IS A HIGHLY SORPTIVE MINERAL
- CLINOPTILOLITE -- FELDSPAR + SiO<sub>2</sub>
- FIELD EVIDENCE SUGGESTS THAT CLINOPTILO-LITE IS NOT STABLE WHEN THE ACTIVITY OF SiO<sub>2</sub> IS IN EQUILIBRIUM WITH QUARTZ
- AS TEMPERATURE INCREASES, THE ACTIVITY OF SiO<sub>2</sub> MUST INCREASE RELATIVE TO QUARTZ SATURATION TO MAINTAIN CLINOPTILOLITE STABILITY

# DISTRIBUTION OF Los Alamos

#### TRIDYMITE, CRISTOBALITE, AND QUARTZ ARE PRESENT IN YUCCA MOUNTAIN

#### TRIDYMITE

- MOST SOLUBLE
- FOUND AT SHALLOW DEPTH
- GENERALLY ASSOCIATED WITH GLASS

#### CRISTOBALITE

- DECREASES WITH DEPTH
- ASSOCIATED WITH CLINOPTILOLITE BELOW THE STATIC WATER LEVEL

#### QUARTZ INCREASES WITH DEPTH



Los Alamos





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#### PLANNED ACHIEVEMENTS

Los Alamos

#### FY 1985

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- DETERMINE PARTICLE CONTENT OF YUCCA MOUNTAIN WATER
- DETERMINE POTENTIAL OF MICROBIOLOGICAL ACTIVITY TO ALTER GROUNDWATER COMPOSITION
- PLAN IN SITU DEMONSTRATION OF MATRIX DIFFUSION AND PARTICULATE TRANSPORT
- FY 1986
  - UPDATE THE GROUNDWATER COMPOSITIONAL MODEL TO INCLUDE PATHWAY TO THE ACCESSIBLE ENVIRONMENT
  - CALCULATE POSSIBLE TRANSPORT OF WASTE ELEMENTS SORBED ON PARTICULATES
  - ESTIMATE PALEOHYDROLOGICAL FLAWS THROUGH ZEOLITIZED ZONES ABOVE THE WATER TABLE AT YUCCA MOUNTAIN
  - START IN SITU TRANSPORT DEMONSTRATION

#### FY 1987

- ESTIMATE TOTAL EFFECTS OF MICROBIOLOGICAL ACTIVITY ON GROUNDWATER COMPOSITION
- PRODUCE UPDATED MODEL OF Eh AND pH BUFFERING CAPACITY OF YUCCA MOUNTAIN TUFF/WATER/AIR SYSTEM





#### ACHIEVEMENTS

- ANALYSIS OF INTEGRAL SAMPLES FROM WELLS USW H-1, H-4, H-5, H-6, G-4, J-13, UE-29a#2, UE-25b#1, AND UE-25p#1
- ANALYSIS OF INDIVIDUAL ZONES FROM WELLS USW H-3, H-6, AND UE-25b#1
- PRELIMINARY MODEL OF GROUNDWATER ALONG PATHWAYS TO ACCESSIBLE ENVIRONMENT, LA-10188-MS
- PRELIMINARY MODEL OF Eh AND pH BUFFERING CAPACITY OF YUCCA MOUNTAIN AREA, LA-10188-MS



- ANALYSIS OF GROUNDWATERS
- TUFF GROUNDWATER INTERACTIONS
- ANALYSIS OF PARTICULATES
- POTENTIAL FOR MICROBIOLOGICAL ACTIVITY
- DEVELOP GROUNDWATER CHEMISTRY MODEL
- MODEL Eh AND pH CAPACITIES OF TUFF/WATER/AIR
- ESTIMATE EFFECTS OF PARTICULATE TRANSPORT
- IN SITU TRANSPORT TEST



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#### WELL-TO-WELL PUMPING TESTS

Los Alamos

#### WELLS UE-25c#1,-2, AND -3

- MEASURE SCALE-SENSITIVE HYDROLOGY PARA-METERS SUCH AS DISPERSION (USGS)
- DEMONSTRATE RETARDATION IN SITU OF NON-SORBING WASTE ELEMENTS, COLLOIDS, AND PARTICULATES IN THE SATURATED ZONE



#### WASTE-ELEMENT MIGRATORS

Los Alamos

•  $95m_{Tc}$   $t^{1/2} = 61 DAYS$ 

- **237**Pu  $t\frac{1}{2} = 45.6$  DAYS
- NATURAL U AND TH ISOTOPES
- FLUORESCENT MICROSPHERES
- ACTINIDE OR RARE-EARTH COLLOIDS



#### Los Alamos

- INTERNAL PLANNING AND REVIEW
- NRC REVIEW AND CONSENT
- COST AND TIMING OF ISOTOPE PRODUCTION
- RADIOLOGICAL HEALTH AND SAFETY

# NN SPROJECT

"ANALYSES AND MODELS THAT WILL BE USED TO PREDICT FUTURE CONDITIONS AND CHANGES IN THE GEOLOGIC SETTING SHALL BE SUPPORTED BY USING AN APPROPRIATE COMBINATION OF SUCH METHODS AS FIELD TESTS, IN SITU TESTS, LABORATORY TESTS WHICH ARE REPRESENTATIVE OF FIELD CONDITIONS, MONITORING DATA, AND NATURAL ANALOG STUDIES."

10CFR60, 60.21 (C) (I) (ii) (F)



Los Alamos

# NATURAL ISOTOPE CHEMISTRY WBS 2.3.4.1.2 A. E. NORRIS

### NN WS I PROJECT

#### MEASUREMENTS OF YUCCA MOUNTAIN SAMPLES TO DETERMINE

• INFILTRATION FROM <sup>36</sup>CI "BOMB PULSE" DATA

Los Alamos

• 99 Tc TRANSPORT RELATIVE TO 36CI

GROUNDWATER RETARDATION OF U, Th, AND Ra



# PARAMETER TO BE MEASURED ● DEPTH OF <sup>36</sup>CI BENEATH SURFACE

#### INFORMATION TO BE OBTAINED • PRECIPITATION INFILTRATION DURING PAST 25 YEARS

NEED

HYDROLOGIC MODEL OF YUCCA MOUNTAIN WATER MOVEMENT



#### NATURAL ISOTOPE CHEMISTRY <sup>36</sup>CI INFILTRATION

Los Alamos

FIELD TRIPS

- FEBRUARY 1984
   CHLORIDE CONCENTRATIONS IN YUCCA MOUNTAIN SOILS
- JUNE 1984

SAMPLED TRENCH AT EXPLORATORY SHAFT SITE SELECTED FRACTURED TUFF SITE

AUGUST 1984
 TRIED TO SAMPLE FRACTURED TUFF SITE



#### PARAMETER TO BE MEASURED

99Tc DISTRIBUTION BENEATH SURFACE RELATIVE TO <sup>36</sup>CI

#### INFORMATION TO BE OBTAINED <sup>99</sup>Tc TRANSPORT IN YUCCA MOUNTAIN SOIL RELATIVE TO <sup>36</sup>CI

NEED

• 99Tc TRANSPORT CALCULATIONS

## NATURAL ISOTOPE Los Alamos CHEMISTRY U, Th, AND Ra RETARDATION

#### **PARAMETERS TO BE MEASURED**

• DISTRIBUTIONS OF  $238_{U_1} 234_{U_2} 234_{Th_2} 232_{Th_2} 230_{Th_2} 228_{Th_2} 228_{Ra_2} 226_{Ra_2} 224_{Ra_2} AND 222_{Rn} IN YUCCA MOUNTAIN ROCK AND WATER SAMPLES$ 

#### **INFORMATION TO BE OBTAINED**

- RETARDATION OF TRANSPORT OF LATER MEMBERS
- **OF CHAINS RELATIVE TO EARLIER MEMBERS**

NEED

• CALCULATION OF RADIOLOGICAL SAFETY IN THE FUTURE FOR THE YUCCA MOUNTAIN NUCLEAR WASTE REPOSITORY



# SOLUBILITY DETERMINATION WBS 2.3.4.1.4 J. F. KERRISK

Los Alamos



**OBJECTIVE OF SOLUBILITY** - Los Alamos DETERMINATION TASK

## DETERMINE SOLUBILITIES AND SPECIATION OF IMPORTANT WASTE ELEMENTS UNDER CONDITIONS THAT ARE CHARACTERISTIC OF THE REPOSITORY AND ALONG FLOW PATHS TO THE ENVIRONMENT



HOW WILL SOLUBILITY AND SPECIATION AFFECT RETARDATION?

- SOLUBILITY AND SPECIATION DATA ARE USED TO CALCULATE WASTE-ELEMENT CONCENTRATIONS:
  - (1) AT THE WASTE AS AN ALTERNATE TO SOLID—WASTE DISSOLUTION RATES (SOURCE TERM)
  - (2) ALONG FLOW PATHS IN RESPONSE TO CHANGING WATER CONDITIONS
- SPECIATION DATA ARE USED TO ESTIMATE HOW CHANGING WATER COMPOSITIONS INFLUENCE SORPTION



REGULATORY BASIS FOR Los Alamos SOLUBILITY DETERMINATION

#### NRC <u>DRAFT</u> TECHNICAL POSITION ON SOLUBILITY – IF SOLUBILITIES ARE USED FOR PERFORMANCE ASSESSMENT, THEY SHOULD BE BASED ON SITE-SPECIFIC EXPERIMENTS UNDER EXPECTED REPOSITORY CONDITIONS

• NRC COMMENTS DURING GEOCHEMISTRY WORKSHOPS



#### SOLUBILITY DETERMINATION Los Alamos APPROACH

#### (1) DETERMINE IMPORTANT WASTE ELEMENTS AND REPOSITORY CONDITIONS

- (2) MEASURE IMPORTANT WASTE-ELEMENT SOLUBILITIES
- (3) MODEL SOLUBILITIES USING EXISTING SPECIATION DATA – IF MODEL IS INADEQUATE, IDENTIFY IMPORTANT AQUEOUS SPECIES AND MEASURE FORMATION CONSTANTS



**SOLUBILITY DETERMINATION** Los Alamos APPROACH (continued)

(4) IDENTIFY IMPORTANT WASTE ELEMENTS FORMING COLLOIDS IN SIGNIFICANT QUANTITIES – CHARAC-TERIZE PHYSICAL AND CHEMICAL NATURE OF COLLOIDS – MODEL, THERMODYNAMICALLY IF POSSIBLE

(5) CALCULATE WASTE ELEMENT SOLUBILITIES AND COLLOID CONCENTRATIONS AS NEEDED TO SUPPORT PERFORMANCE ASSESSMENT

#### SOLUBILITY DETERMINATION - Los Alamos SUBTASKS

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SUBTASK	DESCRIPTION	SCHEDULE
A tara	IDENTIFY RADIONUCLIDES	NOW - 9/85
B	DEFINE CONDITIONS	3/85 - 12/85
C	MEASURE SOLUBILITIES	9/85 - 3/89
D	MODEL SOLUBILITY AND SPECIATION	NOW - 9/89
Ε	MEASURE SPECIATION	NOW - 6/89
F	COLLOIDS	NOW - 3/87
G	FINAL SOLUBILITY CALCULATIONS	3/89 - 6/90
H	TASK MANAGEMENT	NOW - 9/90
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#### SOLUBILITY DETERMINATION Los Alamos SUBTASKS C AND E BREAKDOWN

SUBTASK

2280H

#### DESCRIPTION

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 MEASURE SOLUBILITIES
 9/85 - 3/89

 Pu, Am, Np
 9/85 - 6/88

 U, Th
 3/86 - 3/89

 Ra, Ni, Zr
 9/86 - 9/88

 OTHER WASTE ELEMENTS
 9/86 - 3/89

MEASURE SPECIATION Am (III) - CARBONATE Pu (IV) - CARBONATE OTHER WASTE ELEMENTS

NOW - 6/89 NOW - 3/86 NOW - 9/86 9/86 - 6/89

**SCHEDULE** 

#### NN PAST BAST CONTRIBUTIONS PROJECT

- THERMODYNAMIC DATA ZEOLITES AND WASTE ELEMENTS
- WASTE-ELEMENT SOLUBILITY MEASUREMENTS
   AND CALCULATIONS
- SOLUBILITY-LIMITED DISSOLUTION MODEL FOR WASTE
- PRELIMINARY ASSESSMENT OF KEY RADIO-NUCLIDES

CONTRACTOR AND



#### Los Alamos

# SORPTION AND PRECIPITATION WBS 2.3.4.1.5 K. W. THOMAS

Los Alamos

#### OBJECTIVE

2235

# TO PROVIDE NECESSARY DATA (SORPTION COEFFICIENTS) FOR PREDICTION OF RADIO-

#### NUCLIDE MOVEMENT FROM THE REPOSITORY TO THE ACCESSIBLE ENVIRONMENT


- 1.3.1 ESTIMATES OF AND BOUNDS ON RADIONUCLIDE RETARDATION BY SORPTION PROCESSES
- 1.3.3 BOUNDS ON EFFECTIVE RETARDATION IN DISPERSIVE/DIFFUSIVE/ADVECTIVE TRANSPORT
- 1.3.4 CALCULATED ESTIMATES OF AND BOUNDS ON RADIONUCLIDE RETARDATION ALONG THE HYDROLOGIC FLOW PATHS WITHIN THE REPOSITORY AND BETWEEN THE REPOSITORY AND THE ACCESSIBLE ENVIRONMENT
- 1.4.2 CALCULATED ESTIMATES OF AND BOUNDS ON THE PERFORMANCE OF THE TOTAL WASTE ISOLATION SYSTEM, INCLUDING WASTE PACKAGE RELEASE RATES, GROUNDWATER TRAVEL TIME, RETARDATION OF RADIONUCLIDES, AND THE INTEGRATED RELEASE OF RADIONUCLIDES TO THE ACCESSIBLE ENVIRONMENT AS A FUNCTION OF TIME
- 2.2.4 CALCULATED ESTIMATES OF AND BOUNDS ON THE EFFECTS OF TECTONIC AND CLIMATIC CONDITIONS THAT HAVE REASONABLE POTENTIAL OF OCCURING ON HYDROLOGIC FLOW PATHS, HYDRAULIC PROPERTIES, AND RETARDATION POTENTIAL WITHIN THE REPOSITORY BLOCK AND BETWEEN THE REPOSITORY AND THE ACCESSIBLE ENVIRONMENT
- 2.2.5 CALCULATED ESTIMATES OF AND BOUNDS ON THE RATES AND CONCENTRATIONS OF RADIONUCLIDE RELEASES FROM THE REPOSITORY TO THE ACCESSIBLE ENVIRONMENT RESULTING FROM FUTURE CLIMATIC CONDITIONS AND TECTONISM



## METHOD

#### (1) MEASURE SORPTION COEFFICIENTS AS A FUNCTION OF MINERALOGY

- WATER COMPOSITION
- TEMPERATURE

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- ATMOSPHERE
- WASTE-ELEMENT CONCENTRATION
- WASTE ELEMENT SPECIATION
- PRESENCE OF DRILLING FLUIDS
- MICROBIAL ACTIVITY
- PRESENCE OF PARTICULATES AND COLLOIDS
- (2) EVALUATE DATA USING VARIOUS STATISTICAL METHODS TO CHARACTERIZE SORPTION BEHAVIOR AND TO IDENTIFY ANY IMPORTANT GAPS IN THE DATA BASE
- (3) USING THE KNOWLEDGE GAINED ABOVE, DEVELOP A MODEL TO PREDICT SORPTION AT YUCCA MOUNTAIN



# NODEL DEVELOPMENT

### GOAL IS TO PREDICT SORPTION OF RADIONUCLIDES ALONG THE FLOW PATH FROM THE REPOSITORY TO THE ACCESSIBLE ENVIRONMENT

- MAY HAVE TO BE AN EMPIRICAL MODEL
- MAY ACTUALLY BE COMPOSED OF SEVERAL DIFFERENT MODELS DEPENDING UPON INDIVIDUAL ELEMENT CHEMISTRIES



# STATISTICAL EVALUATION

Los Alamos

- WORK IN CONJUNCTION WITH THE STATISTICS GROUP IN THE ANALYSIS OF OUR SORPTION DATA BASE
- LOOKING FOR:
  - (1) CORRELATION WITH MINERALOGY, SORPTION TIME, ELEMENT CHEMISTRY, etc
  - (2) OBVIOUS GAPS IN DATA
  - (3) IDENTIFICATION, IF POSSIBLE, OF MOST IMPORTANT VARIABLES

## MINERALOGY

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- DATA BASE INCLUDES STUDIES OF MORE THAN 50 TUFF SAMPLES FROM 9 DIFFERENT UNITS OF YUCCA MOUNTAIN
- ZEOLITES HAVE BEEN IDENTIFIED AS PRIMARY SORPTIVE MINERALS FOR SIMPLE CATIONS

#### FUTURE

- NEED TO EXAMINE PURE MINERALS TO HELP IDENTIFY SORBING SPECIES AND SORPTION SITES
- BASED ON PURE MINERAL RESULTS, MAKE PREDICTIONS OF SORPTION FOR VARYING TUFF COMPOSITIONS



#### TO DATE

- WELL J-13 WATER HAS BEEN USED AS "REPRESENTATIVE" WATER FROM YUCCA MOUNTAIN. EXTENSIVE DATA BASE EXISTS
- WELL UE-25p#1 WATER IS BEING INVESTIGATED AS AN EXAMPLE OF HIGH SALT CONTENT YUCCA MOUNTAIN WATER
- WELL H-3 WATER IS BEING INVESTIGATED AS AN EXAMPLE OF HIGH pH YUCCA MOUNTAIN WATER
- DEIONIZED WATER HAS BEEN INVESTIGATED ON NUMEROUS SAMPLES AND GIVES SIMILAR RESULTS AS J-13 WATER

#### FUTURE

• STUDIES OF VADOSE WATER MUST WAIT UNTIL THE EXPLORATORY SHAFT IS COMPLETE AND SAMPLES CAN BE TAKEN

#### IMPORTANT COMPOSITIONAL VARIABLES OF WATER FROM WELLS J-13, UE-25p#1

(1298 TO 1792 m), AND H-3

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		Well	Well UE-25p#1	Well
	Component <sup>a</sup>	J-13	<u>(1293 to 1792 m)</u>	<u>H-3</u>
		•	•	
	рH	7	6.7	9.1
Total	carbonate, mol//	$2.8 \times 10^{-3}$	1.61 x $10^{-2}$	~10 <sup>-3</sup>
	so <sup>=</sup> 4	18.1	129	32
	<b>C1</b>	6.4	37	9.1
	F	2.1	3.5	5.4
	Na <sup>+</sup>	45.2	110	126
	κ+	5.47	13.4	1.73
	Ca <sup>2+</sup>	11.5	87.8	0.79
	Mg <sup>2+</sup>	1.73	31.9	0.015
	SiO <sub>2</sub> (aq)	64.2	37.2	36

<sup>a</sup>Listed in units of mg/l unless otherwise noted.

#### SORPTION RATIOS IN UE-25p#1, J-13, AND DEIONIZED WATERS

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· · · · · · · · · · · · · · · · · · ·			SORPTION RATIOS (ml/g)		
,	CORE	ELEMENT	UE-25p#1	J-13	
<b>GU3–1301</b>		Sr	10(2)	32(8) 160(35) 570(60) 75(12)	
		Cs	45(5)		
		Ba	82(18)		
		Eu	>17 000		
		SORPTION RATIOS (m4/g)			
CORE	ELEMENT	UE-25p#1	J-13	DEIONIZED	
G1-2233	Sr	2 000(330)	48 000(3 000)	>56 000	
	Cs	7 500(1 100)	13 500(800)	13 000(1 600)	
:	Ba	41 000(6 300)	250 000(30 000)	55 000(5 300)	
	Eu	>5 600	900(200)	810(100)	

COMPARISON OF TIN SORPTION RATIOS IN J-13 AND UE-25p#1° GROUNDWATERS Los Alamos

CORE	SORPTIC (ml	on ratios (/g)	DESORPTION RATIOS (ml/g)	
	J-13	UE-25#1	J-13	UE-25#1
G1-2840	283	20000	780	18400
GU3-1301	168	4000	1280	6750
G4-1502	215	800	500	300
G1-2901	22000	35800	38000	52500

"WATER FROM DEPTH 1298-1792m.

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## WASTE-ELEMENT CONCENTRATION

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PAST STUDIES FOR SEVERAL ELEMENTS ON YUCCA MOUNTAIN TUFF SAMPLES INDICATE, ON A GROSS SCALE, THAT THE SORPTION COEFFICIENTS CHANGE LITTLE OVER 7-8 ORDERS OF MAGNITUDE IN ELEMENT CONCENTRATION

> **HOWEVER:** THEY GIVE NO INFORMATION ON THE SORBING SPECIES OR SORPTION SITES

 FUTURE STUDIES WILL BE PERFORMED ON PURE MINERALS AT VARYING pH VALUES TO DETERMINE WHAT SITES ON THE MINERALS (SURFACE OR INTERSTITIAL) ARE RESPONSIBLE FOR SORPTION AND WHICH SPECIES OF THE ELEMENT IN QUESTION ARE ACTUALLY SORBING

	ODDTION DATIOS LINDED				
$CO_2 - CONTROLLED ATMOSPHERIC CONDITIONS$					
√	Los Alam				
Np CONC (M)	SORPTION RATIO (ml/g)				
6 x 10 <sup>-4</sup>	2.4				
3 x 10 <sup>-4</sup>	0.94				
7 x 10 <sup>-5</sup>	3.4				
$3 \times 10^{-5}$	3.3				
8 x 10 <sup>-6</sup>	4.9				
3 x 10 <sup>-6</sup>	5.0				
7 × 10 <sup>-7</sup>	5.0				
$4 \times 10^{-7}$	5.2				
2 x 10 <sup>-11</sup>	5.4				



MULTIVALENT ACTINIDES PRESENT PARTICULARLY DIFFICULT PROBLEMS

- SEVERAL SPECIES MAY BE PRESENT AT NEUTRAL pH
- CONCENTRATION OF THE VARIOUS SPECIES MAY NOT BE CONSTANT AT NEUTRAL pH
- CONCENTRATION LEVELS: OF THE SPECIES BEING STUDIED ARE BELOW DETECTION LIMITS
- WHICH SPECIES WILL BE MOST IMPORTANT WILL BE DETERMINED BY WASTE FORM, CANISTER MATERIAL, BACKFILL MATERIAL, GROUND-WATER CHEMISTRY, etc, MOST OF WHICH ARE CURRENTLY UNDEFINED. THEREFORE, WE MUST CONCENTRATE OUR STUDIES ON THE MOST "PROBABLE" CANDIDATES AS DETERMINED BY CALCULATIONS



- BACTERIA HAVE BEEN ISOLATED FROM YUCCA MOUNTAIN THAT ACTIVELY GROW USING DRILLING POLYMER AS THEIR ONLY FOOD SOURCE
- THESE SAME BACTERIA HAVE BEEN SHOWN TO "SORB" PLUTONIUM FROM WELL J-13 WATER IN THE PRESENCE AND ABSENCE OF YUCCA MOUNTAIN TUFF

• QUESTIONS INCLUDE

(1) CAN THE BACTERIA TRANSPORT THE PLUTONIUM UNDERGROUND ?

- (2) DO BACTERIAL DECAY PRODUCTS ALSO COMPLEX PLUTONIUM ?
- (3) WHAT ROLE DO ANAEROBIC BACTERIA PLAY?

## SEALING MATERIALS EVALUATION WBS 2.4.2.3.2 C. J. DUFFY

## DEVELOP SEALING MATERIALS FOR FRACTURES, BOREHOLES, AND ACCESS SHAFTS AND DRIFTS AND ASSESS THEIR CHEMICAL STABILITY AND POSSIBLE EFFECTS UPON WATER CHEMISTRY



## N N Los Alamos W S PROJECT

1.4.2 CALCULATED ESTIMATES OF AND BOUNDS ON THE PERFORMANCE OF THE TOTAL WASTE ISOLATION SYSTEM, INCLUDING WASTE PACKAGE RELEASE RATES, GROUNDWATER TRAVEL TIME, RETARD-ATION OF RADIONUCLIDES, AND THE INTEGRATED RELEASE OF RADIONUCLIDES TO ACCESSIBLE ENVIRONMENT AS A FUNCTION OF TIME

**3.4.6 DEFINITIONS OF THE METHOD OF BACKFILLING AND SEALING BOREHOLES, DRIFTS, AND SHAFTS** 



WILL THE EFFECTIVENESS OF THE SEALS IN INHIBITING WATER FLOW DECREASE WITH TIME DUE TO MINERALOGIC CHANGES IN THE SEAL OR THE ADJACENT TUFF ?

**CONCERNS** 

WILL INTERACTIONS BETWEEN THE SEALING MATERIAL AND WATER INCREASE THE ABILITY OF THE WATER TO CARRY WASTE ELEMENTS ?



WATER CHEMISTRY

## • IS EMPLACEMENT OF A SEAL LIKELY TO CHANGE THE pH OF THE GROUNDWATER ?

 IMPORTANT BECAUSE SOLU-BILITY OF THE WASTE IS pH DEPENDENT



## WATER CHEMISTRY

- WILL ALTERATION OF THE SEALING MATERIAL ADD COMPLEXING AGENTS TO THE WATER THAT WOULD INCREASE WASTE SOLUBILITY ?
- SULFATE MINERALS ARE USED AS EXPANSIVE
  AGENTS IN SEALING MATERIALS
- WOULD LIBERATION OF THIS SULFATE APPRE-CIABLY INCREASE WASTE TRANSPORT ?



## MECHANICAL PROPERTIES

## PRIMARY PROPERTY OF CONCERN IN SEAL IS PERMEABILITY

## MECHANICAL STRENGTH OF THE SEAL MAY BE OF SECONDARY CONCERN



- IMPORTANT IN SEAL MATERIAL AND ADJACENT TUFF
- MINERAL ALTERATION WILL OCCUR BECAUSE THE TUFF AND SEAL ARE NOT IN EQUILIBRIUM AT THE TIME OF EMPLACEMENT
- MINERAL ALTERATION WILL ALSO OCCUR BE-CAUSE OF CHANGES IN TEMPERATURE DURING REPOSITORY HEATING



### DISEQUILIBRIUM BETWEEN Los Alamos SEAL MATERIAL AND TUFF

- POSSIBLE SEALING MATERIAL COMPOSITION HAS BEEN ADJUSTED TO MAKE IT APPROACH EQUILIBRIUM WITH TUFF
- ACCOMPLISHED PRIMARILY BY ADDITION OF SILICA

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#### TEMPERATURE EFFECTS Los Alamos UPON FAULT AND FRACTURE SEALS

IMPORTANT LOW-TEMPERATURE PHASES ARE CALCIUM SILICATE HYDRATE AND THE EXPANSIVE AGENT ETTRINGITE

• AT 100° TO 150° C

CALCIUM SILICATE HYDRATE --> TOBERMORITE ETTRINGITE --> ANHYDRITE ?

### • ABOUT 200<sup>0</sup> C TOBERMORITE ---> TRUSCOTTITE



- WHY IS IT IMPORTANT?
- CHANGES IN MINERALOGY MAY AFFECT SOLUBILITY
- VOLUME CHANGES MAY ACCOMPANY MINERALOGIC CHANGES AND INCREASE THE PERMEABILITY OF THE SEAL
- CHANGES IN MINERALOGY MAY AFFECT THE CEMENTITIOUS QUALITIES OF THE SEAL MATERIAL AND CHANGE ITS STRENGTH



# SEAL-WATER INTERACTION

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- WATER COMING INTO CONTACT WITH THE SEAL WILL NOT BE IN EQUILIBRIUM WITH IT
- DISSOLUTION AND/OR PRECIPITATION
  MAY OCCUR
- IS SUFFICIENT DISSOLUTION POSSIBLE TO CAUSE FAILURE OF THE SEAL ?



## DISSOLUTION OF FAULT SEALS

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PRELIMINARY DISSOLUTION MODEL FOR FAULT SEALS INDICATES THAT FAULT SEAL DISSOLUTION IS LIKELY TO BE IMPORTANT ONLY IF

- THE BULK PERMEABILITY OF THE SEAL IS GREATLY INCREASED
- THERE IS SHRINKAGE OF THE FAULT SEAL



## **FUTURE WORK**

- FURTHER DEFINE MINERALOGIC CHANGES DUE TO INCREASED TEMPERATURE
- DETERMINE PHYSICAL PROPERTIES FOR ALTERED SEALING MATERIALS
  - BULK PERMEABILITY
  - INTERFACE PERMEABILITY
  - VOLUME CHANGE DUE TO MINERAL ALTERATION
  - BOND STRENGTHS
- **REFINE FAULT SEAL DISSOLUTION MODEL**

DYNAMIC TRANSPORT PROCESS WBS 2.3.4.1.6 R. S. RUNDBERG

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## DYNAMIC TRANSPORT Los Alamos PROCESS

#### 1. CRUSHED ROCK COLUMNS – SPECIATION, KINETICS

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2. FRACTURED TUFF COLUMNS – MATRIX DIFFUSION, CAPILLARY SUCTION

3. SOLID TUFF COLUMNS – SPECIATION, KINETICS, FILTRATION OF PAR-TICULATES, AND CHEMICAL-FLOW COUPLING

- 4. VAPOR PHASE TRANSPORT
- 5. AUXILIARY EXPERIMENTS
  - a. DIFFUSION IN THE ABSENCE OF FLOW
  - **b. PARTICLE SIZE ANALYSES**
  - c. SORPTION KINETICS

## N CRUSHED TUFF COLUMNS

#### PAST ACHIEVEMENTS

• SIMPLE CATIONS Sr<sup>++</sup>, Cs<sup>+</sup>, AND Ba<sup>++</sup> SHOWN TO AGREE WITH BATCH SORPTION MEASUREMENT (PROVIDED PARTICLE SIZE FRACTIONATION WAS CONTROLLED)

#### **RECENT ACHIEVEMENTS**

- PLUTONIUM AND AMERICIUM FOUND TO HAVE A SMALL FRACTION WHICH ELUTES EARLIER THAN HTO (PRELIMINARY RESULTS INDICATE HYDRODYNAMIC CHROMATOGRAPHY)
- 76% Tc 95-m FOUND TO ELUTE AS AN ANION, TcO<sub>4</sub>, ELUTING EARLIER THAN HTO. 24% ADSORBED



CRUSHED TUFF COLUMNS (cont)

**FUTURE WORK** 

- DETERMINE THE IDENTITY OF THE ACTINIDE FRACTION WHICH ELUTES EARLY
  - COMPARE WITH ANIONS
  - COMPARE WITH COLLOID STANDARDS
  - STUDY DEFINED ACTINIDE SPECIES
- DETERMINE THE MECHANISM RESPONSIBLE FOR Tc 95-m ADSORPTION
  - IDENTIFY SPECIES CHARGE
  - STUDY Tc 99 (POSSIBLE AUTORADIOLYSIS)





## FRACTURED TUFF COLUMNS

**Los Alamos** 

## PAST ACHIEVEMENTS

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• NONSORBING TRACER SHOWN TO FIT MATRIX DIFFUSION MODEL

• CONSTRICTIVITY/TORTUOSITY FACTORS OF 0.01 - 0.1

 PRELIMINARY EVIDENCE INDICATES THAT SORPTION IS EFFECTIVELY DECREASED MORE THAN AN ORDER OF MAGNITUDE

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## FRACTURED TUFF COLUMNS (cont)

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**FUTURE WORK** 

 DETERMINE CAUSE OF SORPTION DECREASE
 – UNEVEN DISTRIBUTION OF SORBING MINERALS?
 – CHANNELING?

• PERFORM EXPERIMENTS WITH UNSATURATED COLUMNS

- EXAMINE PARTICULATE TRANSPORT IN FRACTURES
- TEST FLOW TRACERS



## SOLID TUFF COLUMNS

## PAST ACHIEVEMENTS

• Sr SHOWN TO BE IN GOOD AGREEMENT WITH BATCH AND CRUSHED TUFF COLUMN FOR TOPOPAH SPRING TUFF SAMPLE

## **FUTURE WORK**

- UNSATURATED FLOW
- FILTRATION OF COLLOIDS
- GEOCHEMICAL FLOW COUPLING
- CATIONS CONTINUED


#### PAST ACHIEVEMENTS

• EARLY RESULTS FROM TUFF WAFERS INDICATE CONSTRIC-TIVITY/TORTUOSITY FACTOR FROM 0.1 TO ~1.0

#### **FUTURE WORK**

- DETERMINE IF DIFFUSION COEFFICIENTS ARE SUBJECT TO SCALING EFFECTS
- DETERMINE DIFFUSIVITIES IN TUFF FOR IMPORTANT WASTE ELEMENTS
- DETERMINE DIFFUSIVITY AS A FUNCTION OF SATURATION

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# PARTICLE SIZE ANALYSIS

ACCOMPLISHMENTS

• DEVELOPMENT OF A "STATE-OF-THE-ART" AUTO-CORRELATOR SPECTROMETER

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• DETERMINED THE SIZE DISTRIBUTION BY APS OF PLUTONIUM POLYMER IN pH 8 WATER

## FUTURE WORK

- DETERMINE THE RESOLUTION LIMITS OF APS
- DETERMINE ACTINIDE SIZE DISTRIBUTIONS, FOR ACTINIDE COLLOIDS UNDER VARIOUS CONDITIONS
- DEVELOP NONINTERACTING COLLOID TRACERS



# SORPTION KINETICS

# ACCOMPLISHMENTS

# ION EXCHANGE OF SIMPLE CATIONS IN TUFF SHOWN TO BE DIFFUSION LIMITED (2 STEP DIFFUSION)

## FUTURE WORK

• KINETICS OF SORPTION OF THE ACTINIDES



# NNN SI PROJECT

# RETARDATION SENSITIVITY ANALYSIS WBS 2.3.4.1.7 B. J. TRAVIS

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### SCHEDULE

SUBTASK A: BENCHMARKING COMMENCE: IN PROGRESS COMPLETE: SEPTEMBER 1986

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- SUBTASK B: DIFFUSION CALCULATIONS COMMENCE: IN PROGRESS COMPLETE: APRIL 1985
- SUBTASK C: COUPLED PHENOMENA COMMENCE: IN PROGRESS COMPLETE: APRIL 1985
- SUBTASK D: FRACTURE-FLOW EXPERIMENT COMMENCE: IN PROGRESS COMPLETE: MARCH 1985
- SUBTASK E: GEOCHEMICAL TRANSPORT CALCULATIONS COMMENCE: IN PROGRESS COMPLETE: SEPTEMBER 1985

- SUBTASK F: ALTERNATE NUMERICAL METHODS COMMENCE: IN PROGRESS COMPLETE: SEPTEMBER 1985
- SUBTASK G: PARTICULATE TRANSPORT COMMENCE: IN PROGRESS COMPLETE: SEPTEMBER 1986
- SUBTASK H: HEAT-LOAD EFFECTS COMMENCE: IN PROGRESS COMPLETE: SEPTEMBER 1985
- SUBTASK I: STOCHASTIC METHODOLOGY COMMENCE: JANUARY 1985 COMPLETE: JANUARY 1986
- SUBTASK J: SENSITIVITY ANALYSIS COMMENCE: MARCH 1985 COMPLETE: JUNE 1987
- SUBTASK K: DATA INTEGRATION COMMENCE: IN PROGRESS COMPLETE: MARCH 1990

#### UNSATURATED HYDROTHER- Los Alamos MAL FLOW AND TRANSPORT MODELS LOS ALAMOS

CAPABILITIES

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Michis Michiller;

WAFE – UNSATURATED HYDROTHERMAL FLOW, VAPOR AND LIQUID TRACR3D – UNSATURATED FLOW, TRANSPORT OF PARTICULATES, SOLUBILITY LIMITS, KINETICS TRANQL – FLOW WITH TRUE GEOCHEMISTRY

DEVELOPMENTS

TRANOL – ADDITION OF PRECIPITATION/SOLUBILITY CHEMISTRY WAFE/TRACR3D – COUPLING WITH EQ3/6 INVADJC – SENSITIVITY CALCULATIONS

**APPLICATIONS** 

- TRANSPORT IN "COATED" FRACTURES
- PARTICULATE/COLLOID TRANSPORT
- HYDROTHERMAL CIRCULATION
- COUPLED PHENOMENA
- SENSITIVITY/UNCERTAINTY ANALYSIS
- COMPARISON OF GEOCHEMICAL vs Kr TRANSPORT
- EXPERIMENTAL DESIGN



# INTERACTION BETWEEN Los Alamos MODELS AND EXPERIMENTS

# MODEL VALIDATION, INTERPRETATION

EXPERIMENT -

PREDICTION, DESIGN

# MATHEMATICAL Los Alamos CHARACTERIZATION

DETERMINISTIC

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W S MARSH SHOW

- FORWARD REQUIRES SPECIFICATION OF SPATIAL DISTRIBUTION OF PROPERTIES, b.c.s., i.c.s.
- INVERSE TWEAKING NO JUSTIFICATION OF SOLUTION FORMAL – CAN ACCOUNT FOR MEASUREMENT ERRORS, GIVES DEGREE OF RESOLUTION

#### STOCHASTIC

- FORWARD REQUIRES SPECIFICATION OF CORRELATION FUNCTIONS – MORE REALISTIC, ALLOWS FOR UNCERTAINTIES – ASSOCIATES ERROR BAR WITH SOLUTIONS
- INVERSE GENERATES CORRELATION FUNCTIONS – ASSOCIATES PROBABILITY TO SOLUTION



RESULTS OF TRACR3D CAL-CULATIONS FOR EXPLORATORY

Los Alamos

SHAFT DIFFUSION TESTS











the first of 17.9





#### LEGEND FOR COLUMN EXPERIMENT

$\overline{\lambda} = 10$ cm <sup>-1</sup>	$\sigma = 20$
$\overline{\lambda} = 20 \text{ cm}^{-1}$	$\sigma = 2.0$
$\overline{\lambda} = 30$ cm <sup>-1</sup>	σ = 15
Model result	
Experimental da	ta





# RESULTS FROM (TRANQL) THAT COMPUTES TRUE GEOCHEMICAL TRANSPORT AS OPPOSED TO K<sub>d</sub> MODELING

THIS MODEL IS BEING ADAPTED TO HANDLE GEOCHEMISTRY APPROPRIATE FOR YUCCA MOUNTAIN







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#### 2230H - Los Alamos PRO С Relative T = 40 Days EDTAAQ 10-6 ---- TRANQL:3 ---- Kd=8.0x10-5 10-7 10-0 Cdaq 10-9 10-10 4 X, m 2 6 6 10 0

 $\gamma = \pm 1$ 



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- 40 Days



# **RESULTS OF TRACR3D CAL-CULATIONS IN SUPPORT OF FRACTURE FLOW EXPERIMENTS**

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NUMERICAL RESULTS OF PRESSURE-DRIVEN - LOS Alamos FRACTURE-FLOW EXPERIMENT WHEN NO PRESSURE IS APPLIED TO SOURCE REGION

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#### FRACTURE-FLOW EXPERIMENT ---- Los Alamos IN WELDED TOPOPAH SPRINGS MEMBER





# TYPICAL WAFE CALCULATION

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THIS IS A SIMULATION OF HEAT LOAD EFFECTS ON

**FLOW IN YUCCA MOUNTAIN** 



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