U.S. DEPARTMENT OF ENERGY
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

PRESENTATION TO THE NUCLEAR WASTE TECHNICAL REVIEW BOARD

SUBJECT: METHODOLOGY FOR VALIDATION OF MODELS

PRESENTER: CHARLES F. VOSS

PRESENTER'S TITLE AND ORGANIZATION: STAFF SCIENTIST
GEOSCIENCES DEPARTMENT
BATTELLE PACIFIC NORTHWEST LABORATORIES

PRESENTER'S TELEPHONE NUMBER: (509) 376-5896

MAY 16-17, 1989

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SCOPE OF PRESENTATION

- DISCUSS THE NEED FOR A VALIDATION METHODOLOGY
- DESCRIBE THE COMPONENTS OF THE VALIDATION METHODOLOGY
- PROVIDE AN EXAMPLE OF THE METHODOLOGY
- IMPLEMENTATION OF THE METHODOLOGY

VALIDATION METHODOLOGY FOR PERFORMANCE ASSESSMENT MODELS

- THE LICENSING RECORD MUST ADDRESS THE APPROPRIATENESS AND QUALITY OF THE DATA USED TO DERIVE THE PREDICTIVE MODELS AND THE LOGIC INVOLVED IN ARRIVING AT THE FINAL MODEL(S)

- THE VALIDATION METHODOLOGY ATTEMPTS TO PROVIDE A SYSTEMATIC APPROACH FOR DOCUMENTING THE DEVELOPMENT AND VALIDITY OF A MODEL WITH A COMMON SET OF PRINCIPLES AND WORKING RULES TO ACHIEVE MODELS OF A MORE UNIFORM QUALITY

- A DRAFT METHODOLOGY HAS BEEN COMPLETED AND IS CURRENTLY BEING REVIEWED WITHIN THE OCRWM PROGRAM

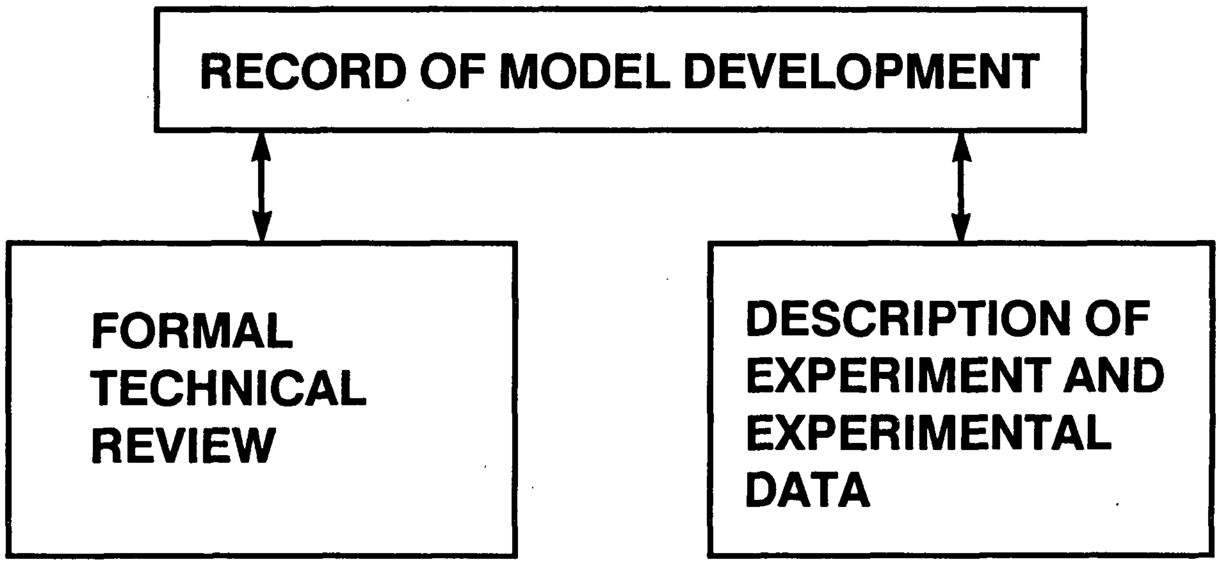
COMPONENTS OF THE METHODOLOGY

1. A RECORD OF THE DERIVATION OF THE MODEL, THE PREMISES UPON WHICH IT IS BASED, AND EVIDENCE TO SUPPORT THESE.

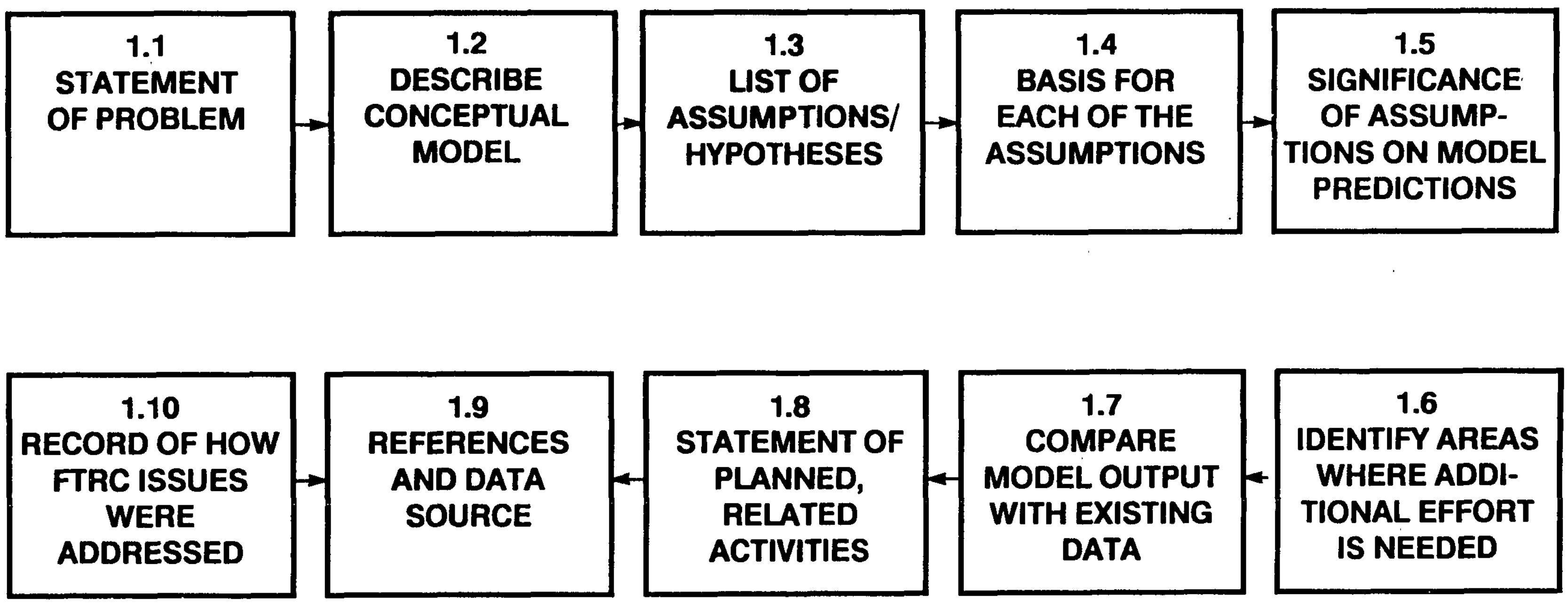
2. A DESCRIPTION OF THE LABORATORY, FIELD, AND NATURAL ANALOG EXPERIMENTS PERFORMED TO SUPPORT MODEL DEVELOPMENT AND TO PROVIDE A COMPARISON BETWEEN EXPERIMENTAL DATA AND MODEL PREDICTIONS.

3. FORMAL TECHNICAL REVIEWS OF 1 AND 2 TO ACHIEVE MODELS OF A MORE UNIFORM QUALITY.

SCHEMATIC OF MODEL VALIDATION METHODOLOGY



RECORD OF MODEL DEVELOPMENT



DESCRIPTION OF EXPERIMENT AND EXPERIMENTAL DATA

2.1
DESCRIPTION OF EXPERIMENT

↓

2.2
INTERPRETATION OF DATA

↓

2.3
COMPARISON OF MODEL OR SUB-MODEL PREDICTION WITH EXPERIMENTAL DATA

FORMAL TECHNICAL REVIEW

Future agenda
Not now in effect

3.1
IDENTIFY MEMBERS OF THE REVIEW COMMITTEE

↓

3.2
DIVIDE MATERIAL INTO FUNCTIONAL ELEMENTS

↓

3.3
ASSIGN ELEMENTS TO REVIEW COMMITTEE MEMBERS

↓

3.4
HOLD REVIEW(S) MODEL AUTHOR(S) EXPLAIN MODEL DEVELOPMENT

↓

3.5
ISSUE REPORT IDENTIFYING REMAINING TECHNICAL ISSUES

APPLICATION OF VALIDATION METHODOLOGY

PURPOSE:

- DEMONSTRATE PROPOSED VALIDATION METHODOLOGY
  - EXAMPLE: MODELING OF RADIONUCLIDE RELEASE FROM EBS
  - EXAMPLE WILL FOCUS ON ONE ASSUMPTION THAT DETERMINES THE CONCEPTUAL AND MATHEMATICAL FORM OF THE RELEASE MODEL
    - * CONGRUENT RELEASE OF RADIONUCLIDES FROM SPENT FUEL UO_2 MATRIX
  - AND AN EXPERIMENT TO TEST THE ASSUMPTION

RECORD OF MODEL DEVELOPMENT

1.1 STATEMENT OF PROBLEM BEING ADDRESSED

- EBS RELEASE OF RADIONUCLIDES ASSUMING SPENT FUEL AS WASTE FORM

- CONCERN: CONSEQUENCES OF UNEXPECTED CONDITIONS (SIGNIFICANT WATER CONTACT WITH SPENT FUEL)

- MECHANISM OF RELEASE (CONGRUENT OR INCONGRUENT) OF RADIONUCLIDES FROM UO_2 MATRIX MAY SIGNIFICANTLY AFFECT COMPLIANCE WITH 10 CFR 60.113

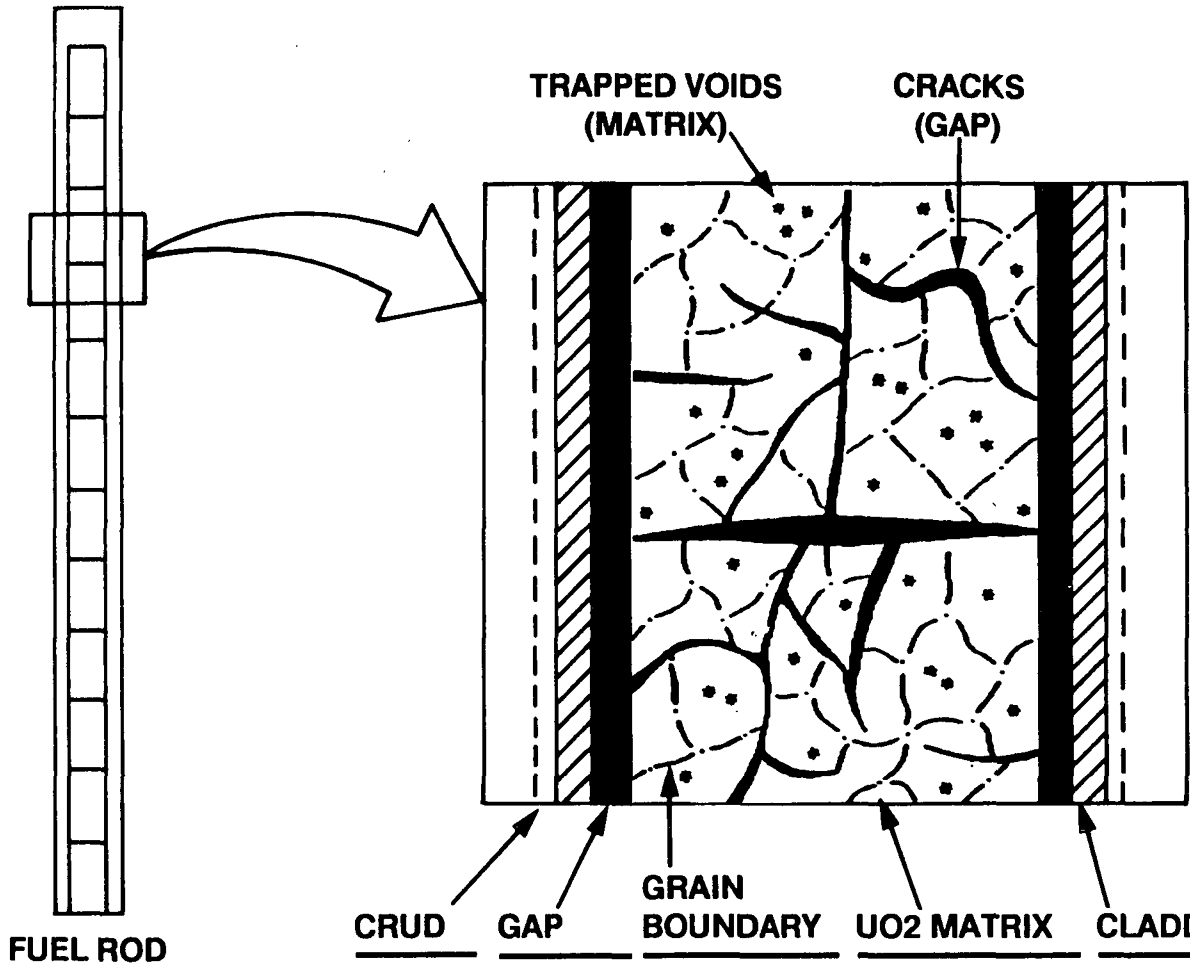
RECORD OF MODEL DEVELOPMENT

1.2 CONCEPTUAL MODEL DESCRIPTION - - FOUR COMPONENTS OF SPENT FUEL AFFECT RELEASE

REFERENCES: JOHNSON, ET AL. 1985, APTED, ET AL. 1987

- CLADDING AND CRUD LAYERS
- FUEL/CLADDING GAP
- GRAIN BOUNDARIES
- UO_2 MATRIX (>98% OF FISSION PRODUCTS)

SCHEMATIC OF SPENT NUCLEAR FUEL



CRUD	GAP	GRAIN BOUNDARY	UO2 MATRIX	CLADDING
C-14	C-14	C-14	ACTINIDES	C-14
	I-129	1-129	~98% FISSION	
	Cs-135	Cs-135	PRODUCTS	
	Ca-137	CS-137		
	Se-79	Se-79		
	Tc-99	Tc-99		
	Sr-90	Sr-90		

RECORD OF MODEL DEVELOPMENT

1.2 CONCEPTUAL MODEL DESCRIPTION

- **IMPORTANT VARIABLES AND PARAMETERS**
  - TEMPERATURE
  - GROUND-WATER CHEMISTRY pH
  - INITIAL CHEMICAL STATE OF FUEL
  - GROUND-WATER FLOW RATES

RECORD OF MODEL DEVELOPMENT

1.2 CONCEPTUAL MODEL DESCRIPTION

- CONGRUENT/INCONGRUENT DISSOLUTION ASSUMPTION AFFECTS MODEL:

  * CONGRUENT: SLOWER RELEASE OF SOLUBLE NUCLIDES
    $RATE_I = R(MATRIX) * X_I$

  * INCONGRUENT: LARGE RELEASES OF SOLUBLE NUCLIDES
    $RATE_I = C_I(SAT) * FLOW$

    USED TO CALCULATE GAP AND GRAIN BOUNDARY RELEASES

    NO CONSENSUS OF WHAT EXPERIMENTAL EVIDENCE SHOWS

RECORD OF MODEL DEVELOPMENT

1.3 IDENTIFICATION OF ASSUMPTIONS AND HYPOTHESES

- PHYSICOCHEMICAL PROCESSES
  (FOR THIS PRESENTATION - FOCUS ON ONE ASSUMPTION)

  * CONGRUENT DISSOLUTIONING OF RADIONUCLIDES IN UO_2 MATRIX

RECORD OF MODEL DEVELOPMENT

1.4 TECHNICAL BASIS FOR ASSUMPTIONS

- CONGRUENT DISSOLUTIONING OF RADIONUCLIDES IN MATRIX
  - PROFESSIONAL JUDGMENT
  - SOME DATA - INTERPRETATION AMBIGUOUS

RECORD OF MODEL DEVELOPMENT

1.5 DISCUSSION AND QUANTIFICATION OF ASSUMPTION

- ASSUMPTION IS A SWITCH: DETERMINING WHICH MODEL TO USE
- WHAT IS IMPACT ON RELEASE CALCULATION UNDER IN-CONGRUENT DISSOLUTION FOR SOLUBLE RADIONUCLIDES?
  - FAILURE TO MEET 10^{-5} FRACTIONAL RELEASE RATES
- PERFORM EXPERIMENT TO DETERMINE IF RELEASE IS CONGRUENT

RECORD OF MODEL DEVELOPMENT

1.6 IDENTIFICATION OF ASSUMPTIONS WHERE ADDITIONAL SUPPORT INFORMATION NEEDED

- ASSUMPTION OF CONGRUENT DISSOLUTION OF SPENT FUEL MATRIX
  - NO UNAMBIGUOUS EVIDENCE THAT IT HOLDS
  - MODEL RESULTS ARE VERY SENSITIVE TO THIS ASSUMPTION

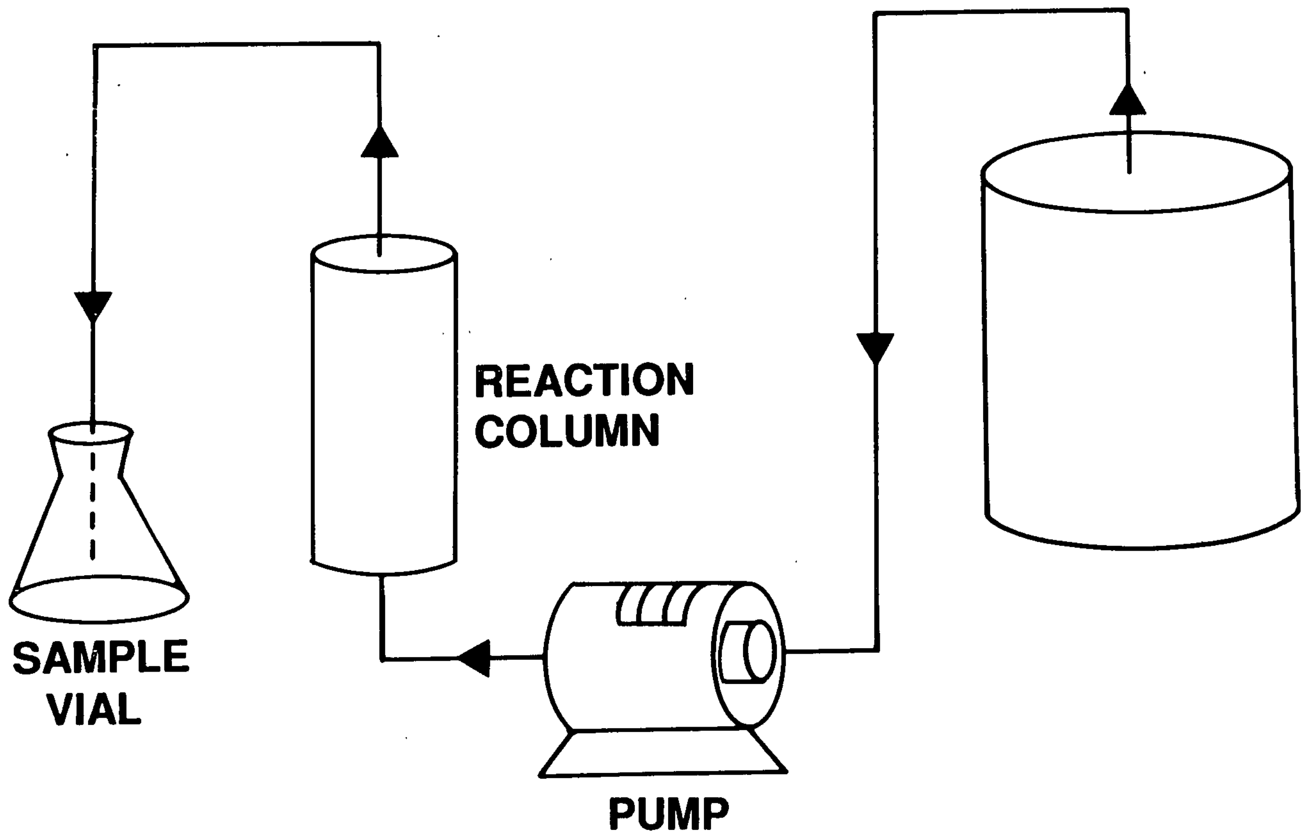
DESCRIPTION OF EXPERIMENT

OBJECTIVE: TEST HYPOTHESIS THAT DISSOLUTION OF THE SPENT FUEL WILL BE CONGRUENT

EXPERIMENTAL DESIGN:

- OXIDIZE FUEL AT 150 °C IN AIR
- CRUSH OXIDIZED FUEL TO PRODUCE INDIVIDUAL GRAINS
- DISSOLVED EXPOSED GRAIN BOUNDARY MATERIAL
- DETERMINE GRAIN BOUNDARY INVENTORY
- LEAVE UNALTERED UO_2 MATRIX AND CONTAINED RADIONUCLIDES
- MEASURE DISSOLUTION RATE OF UO_2 MATRIX AND CONTAINED RADIONUCLIDES

CONGRUENT DISSOLUTION APPARATUS



SOLVENT RESERVOIR

- DEIONIZED WATER
- J13 WELL WATER
- WATER SATURATED WITH URANIUM
- ANOXIC WATER

DESCRIPTION OF EXPERIMENT AND EXPERIMENTAL DATA

2.1 DESCRIPTION OF EXPERIMENT

- NUMBER OF TESTS NEEDED TO EVALUATE HYPOTHESIS
- SOURCES OF VARIATION:
  - NON-HOMOGENEITY OF FUEL (NO QUANTITATIVE ESTIMATE)
  - NON-UNIFORM EFFECTS OF OXIDATION (NO QUANTITATIVE ESTIMATE)
  - ANALYTICAL ERROR ($\pm$ 10%)

DESCRIPTION OF EXPERIMENT AND EXPERIMENTAL DATA

2.2 INTERPRETATION OF DATA

- BECAUSE OF SOURCES OF VARIATION:

  - WITH ABOVE ANALYTICAL ERROR, ASSUMING RATIO IS 1.0, OBSERVABLE RATIO RANGE IS .80

  - ASSUMING GAUSSIAN DISTRIBUTION:
    * FOR 3 TESTS, s(STANDARD DEVIATION) = .47
    * FOR 5 TESTS, s = .34
    * FOR 9 TESTS, s = .27

  - ASSUME WITH ALL SOURCES OF VARIATIONS, s = .80

DESCRIPTION OF EXPERIMENT AND EXPERIMENTAL DATA

2.3 COMPARISON OF MODEL PREDICTION WITH EXPERIMENTAL DATA

- HYPOTHESIS TEST FOR MEAN OF GAUSSIAN POPULATION:

$\frac{\overline{X}-\mu}{s/\sqrt{n}} = t$, COMPARE TO $t_a(n-1)$

$\overline{X}$ - **MEAN OF OBSERVED RATIOS**
μ - **TRUE RATIO VALUE**
n - **NUMBER OF TESTS**
a - **CONFIDENCE LEVEL**

WITH $\overline{X} = 2,\ \mu = 1,\ s = .80,\ n = 3,\ a = .05$

$t = 2.17 < t_a(2)$

IF MEAN RATIO $\leq$ 2, THEN CONGRUENT DISSOLUTIONING CONFIRMED

DESCRIPTION OF EXPERIMENT AND EXPERIMENTAL DATA

2.3 COMPARISON OF MODEL PREDICTION WITH EXPERIMENTAL DATA

- **VIEWING HYPOTHESIS AS TOLERANCE INTERVAL ON INDIVIDUAL RATIOS:**

  - WITH 95% CONFIDENCE, THAT 95% OF POPULATION OF OBSERVED RATIOS $\leq$ LIMIT

  - LIMIT = $\bar{X}$ + K(.95, .95, n)
    FOR N = 5, s = .80, X = 1.0
    LIMIT = 4.37

  - IMPLICATION: SMALL PROBABILITY THAT OBSERVED RATIO > 4.37

RECORD OF MODEL DEVELOPMENT

1.7 COMPARISON OF MODEL OUTPUT AND EXPERIMENTAL DATA FROM HYPOTHESIS OF CONGRUENT DISSOLUTION:

$$H_0: \frac{\text{Cs/U IN SOLUTION}}{\text{Cs/U IN MATRIX}} = 1.0$$

$$H_1: \frac{\text{Cs/U IN SOLUTION}}{\text{Cs/U IN MATRIX}} > 1.0$$

RECORD OF MODEL DEVELOPMENT

1.8 RELATED PLANNED ACTIVITIES

- DYNAMIC DISSOLUTION EXPERIMENTS

  - DETERMINE EFFECTS OF IMPORTANT PARAMETERS FOR RELEASE MODEL:

    * RANGE OF TEMPERATURES

    * RANGE OF WATER COMPOSITIONS

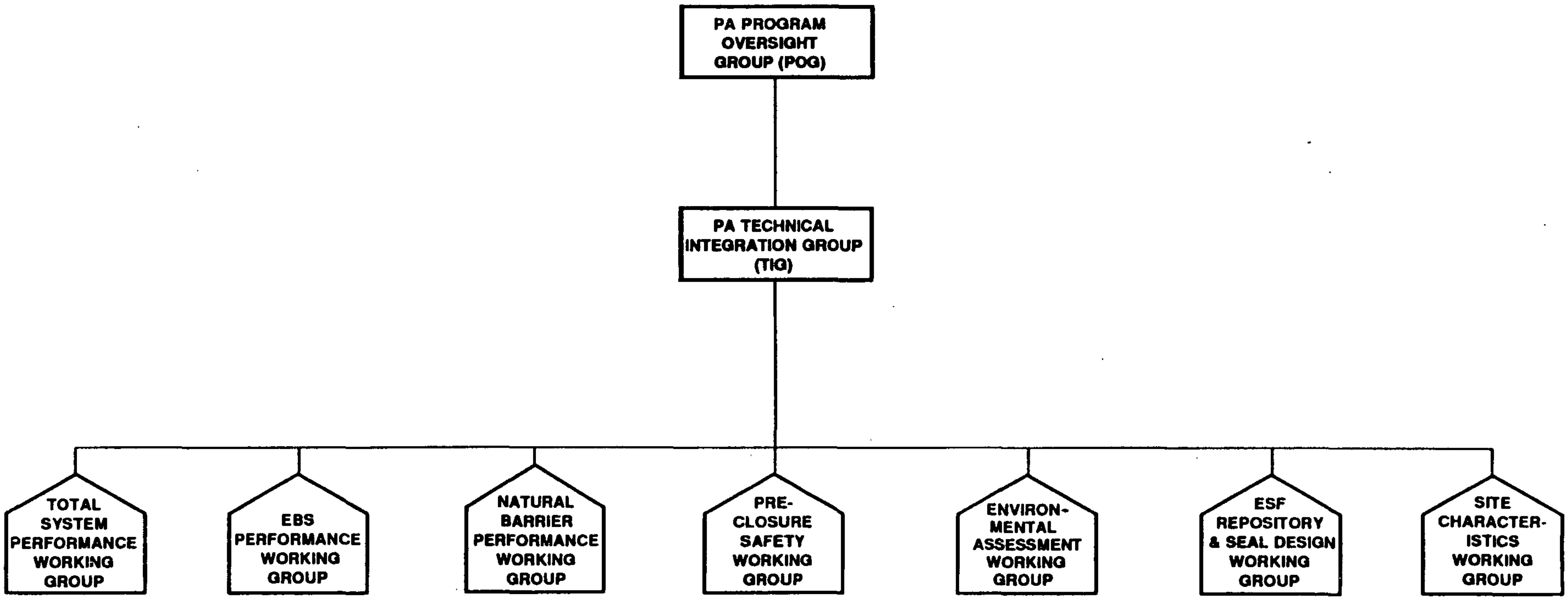
    * RANGE OF OXIDATION STATES OF FUEL

    * EFFECT OF LOW FLOW RATES (USE OF WATER SATURATED WITH U)

IMPLEMENTATION OF MODEL VALIDATION METHODOLOGY

- WORKING GROUP 7 WILL ACT AS THE LEAD FOR INTEGRATING THE METHODOLOGY WITHIN OCRWM
- A SET OF MORE DETAILED EXAMPLES OF THE METHODOLOGY IS BEING PREPARED IN EACH OF THE PERFORMANCE ASSESSMENT AREAS TO ILLUSTRATE THE CONCEPTS
- THE OCRWM PROGRAM IS PARTICIPATING IN THE INTRAVAL PROGRAM, AN INTERNATIONAL COOPERATIVE EFFORT IN THE AREA OF MODEL VALIDATION

PERFORMANCE ASSESSMENT INTEGRATION STRUCTURE



INTRAVAL TEST CASES

1a Radionuclide migration through clay samples by diffusion and advection based on laboratory experiments performed at Harwell, U.K.

1b Uranium migration in crystalline bore cores based on experiments performed at PSI, Switzerland.

2 Radionuclide migration in single natural fissures in granite, based on laboratory experiments performed at KTH.

3 Tracer tests in a deep basalt flow top performed at the Hanford reservation, Washington, USA.

4 Flow and tracer experiments in crystalline rock base on the Stripa 3-D experiment performed within the International Stripa Project.

5 Tracer experiments in a fracture zone at the Finnsjön research area, Sweden.

6 Synthetic data base, based on single fracture migration experiments in Grimsel Rock Laboratory in Switzerland.

7a Redox-front and radionuclide movements in an open pit uranium mine. Natural analogue studies at Poços de Caldas (Minas Gerais), Brazil.

7b Morro do Ferro colloid migration studies. Natural analogue studies at Poços de Caldas (Minas Gerais), Brazil.

8 Natural analogue studies at the Koongarra site in the Alligator Rivers area of the Northern Territory, Australia.

9 Radionuclide migration in a block of crystalline rock based on laboratory experiments performed at AECL, Canada.

10 Evaluation of unsaturated flow and transport in porous media using an experiment with migration of a wetting front in a superficial desert soil performed within a U.S. NRC trench study at Las Cruces, New Mexico.

11 Evaluation of flow and transport in unsaturated fractured rock using studies at the U.S. NRC Apache Leap Tuff Site, near Superior, Arizona.

12 Experiments with changing near-field hydrologic conditions in partially saturated tuffaceous rocks performed in the G-Tunnel Underground Facility at the Nevada Test Site, performed by the Nevada Nuclear Waste Investigation Project of the U.S. DOE.

13 Experimental study of brine transport in porous media performed at RIVM, the Netherlands.

14a Pumping test in highly saline groundwater performed at the Gorleben site.

14b Saline groundwater movements in an erosional channel crossing the salt dome at the Gorleben site.