

**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**

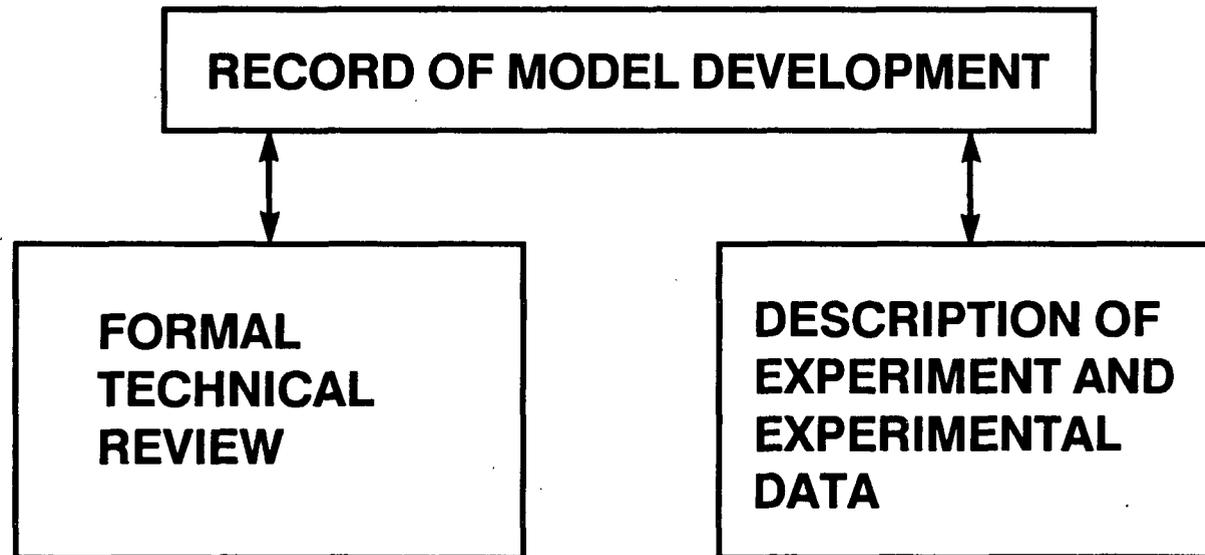
VALIDATION METHODOLOGY FOR PERFORMANCE ASSESSMENT MODELS

- **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**

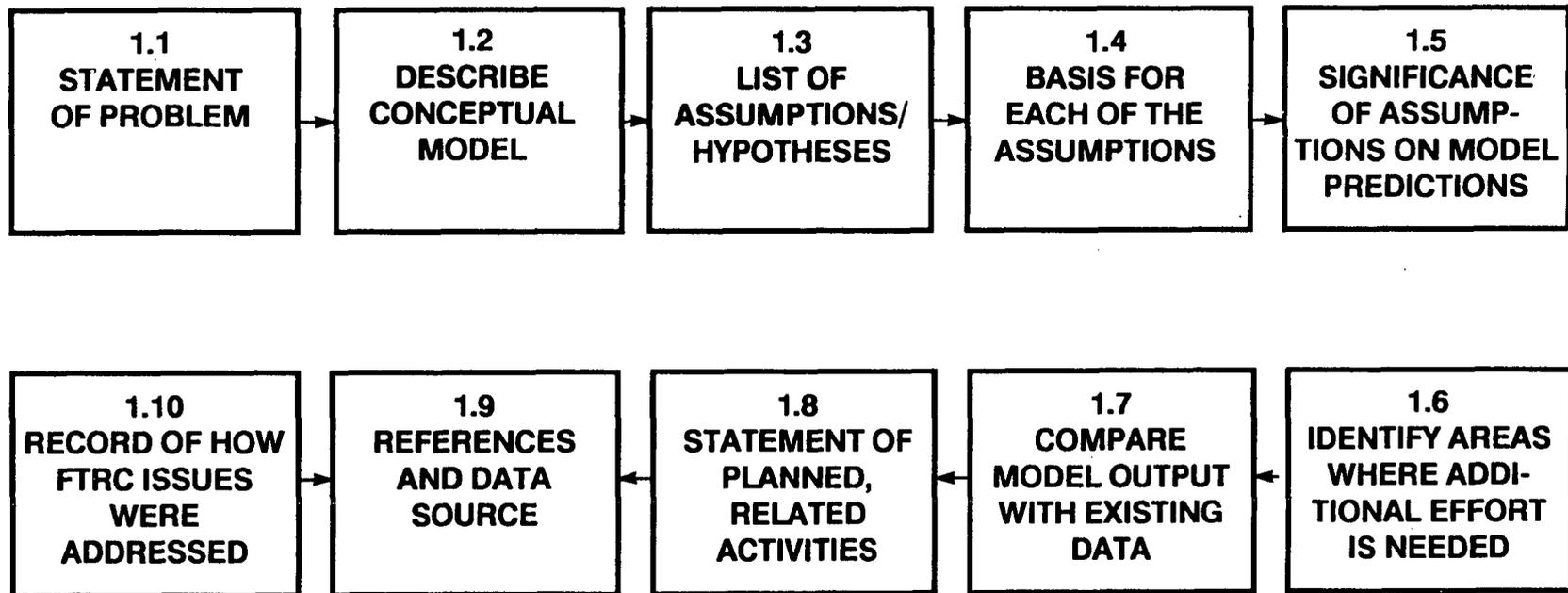
COMPONENTS OF THE METHODOLOGY

- 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.**

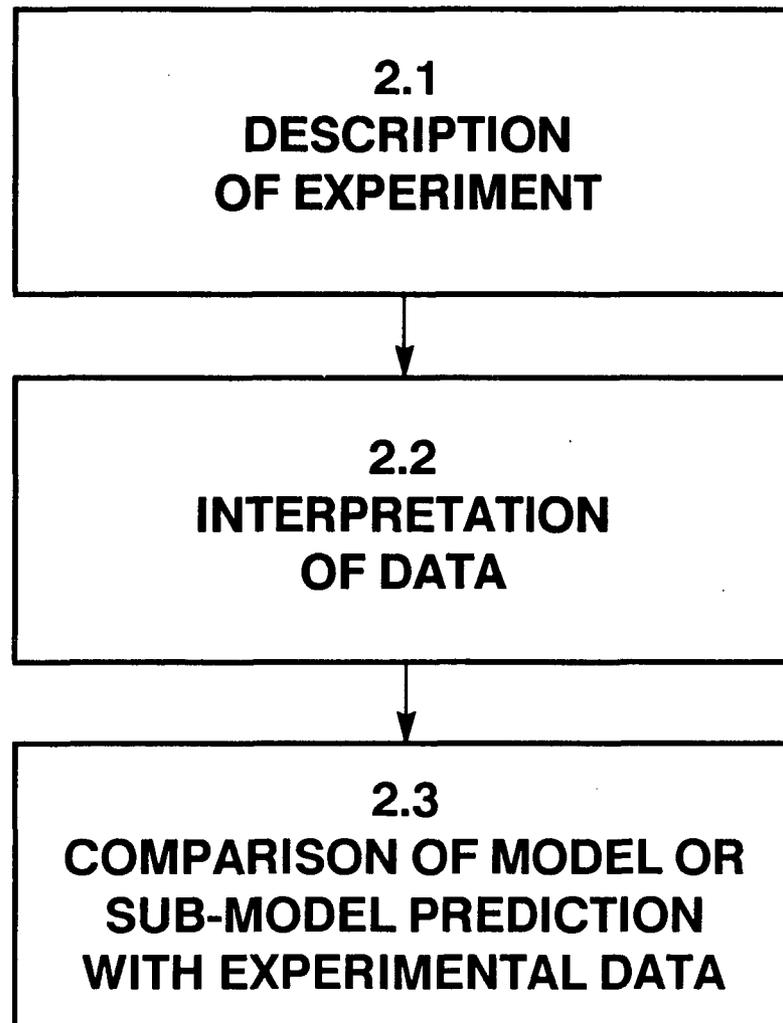
SCHEMATIC OF MODEL VALIDATION METHODOLOGY



RECORD OF MODEL DEVELOPMENT

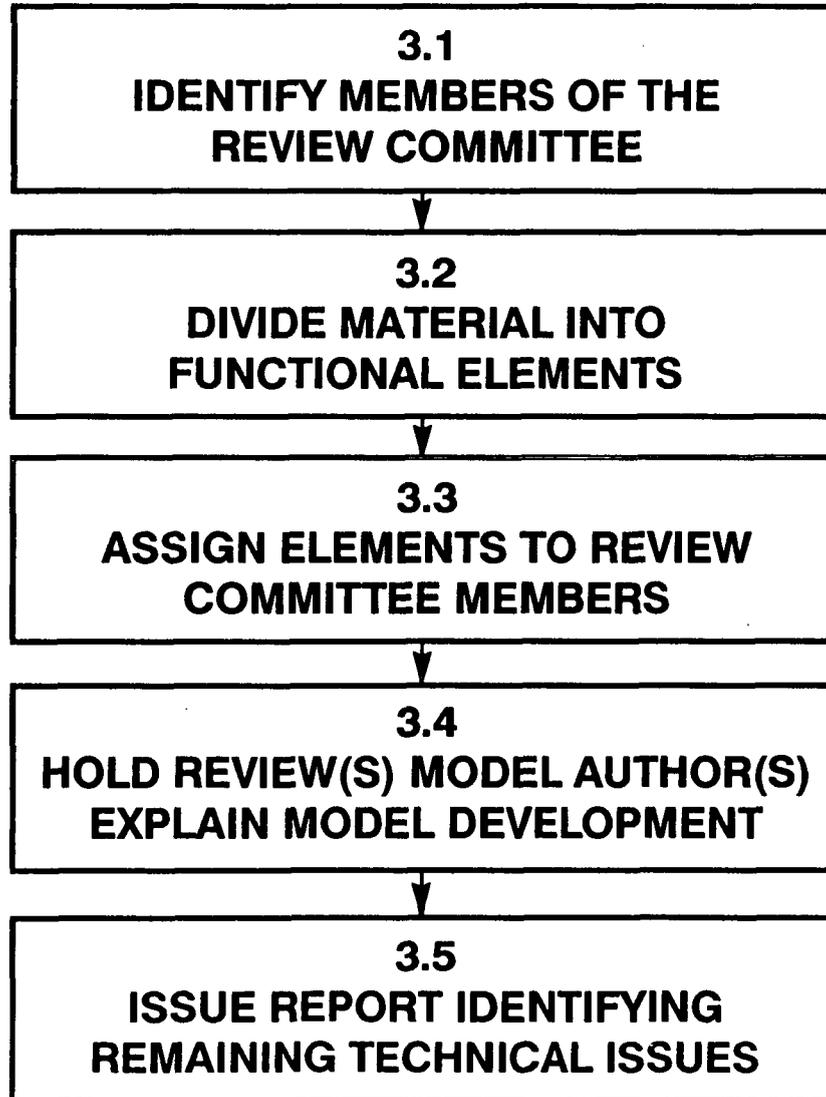


DESCRIPTION OF EXPERIMENT AND EXPERIMENTAL DATA



FORMAL TECHNICAL REVIEW

*Future
Agenda
Not now
in effect*



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**

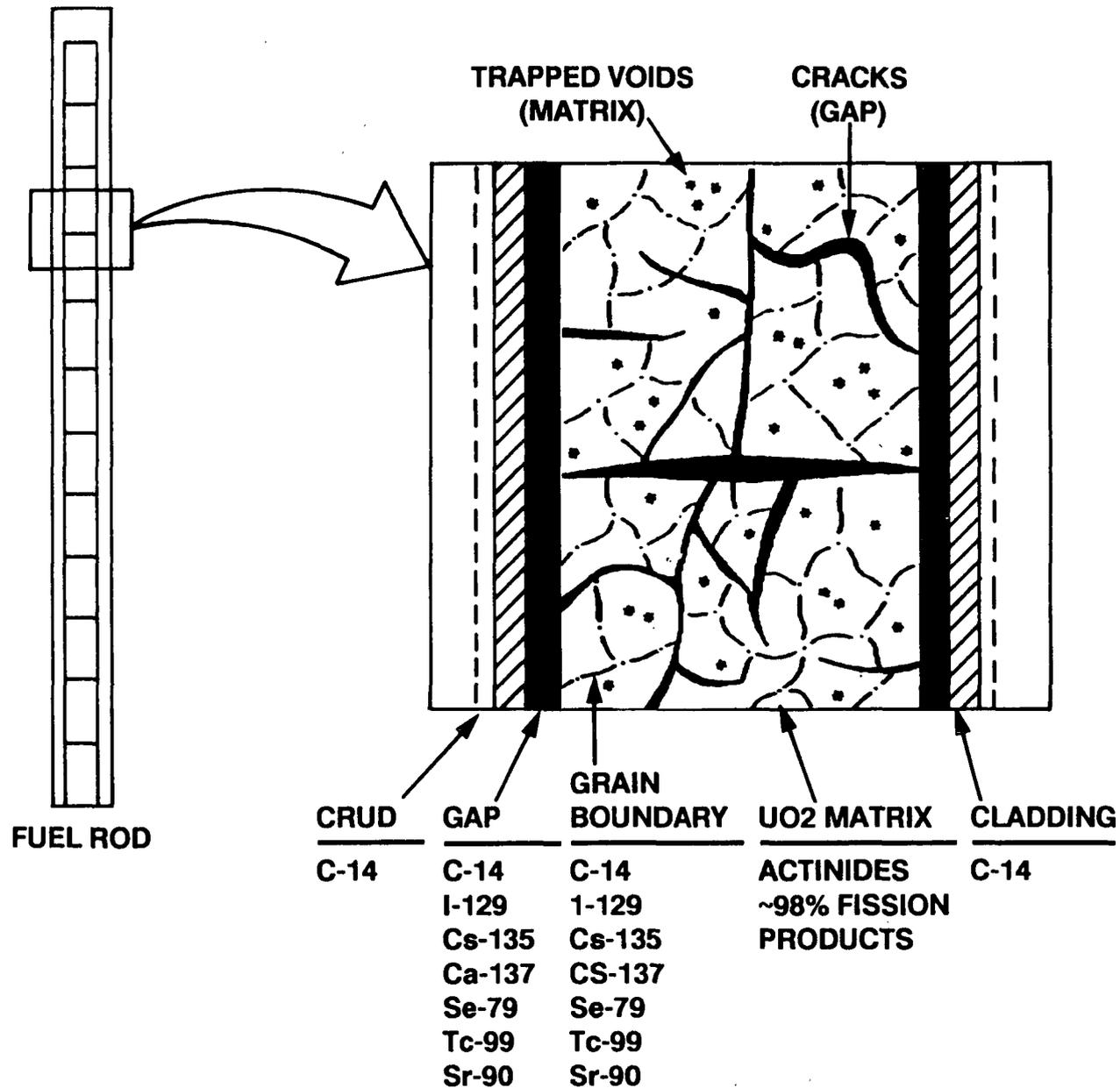
RECORD OF MODEL DEVELOPMENT

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**
- UO₂ MATRIX (>98% OF FISSION PRODUCTS)**

SCHEMATIC OF SPENT NUCLEAR FUEL



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
 $\text{RATE}_i = R(\text{MATRIX}) * X_i$

* INCONGRUENT: LARGE RELEASES OF SOLUBLE NUCLIDES
 $\text{RATE}_i = C_i(\text{SAT}) * \text{FLOW}$

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
UO₂ 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**

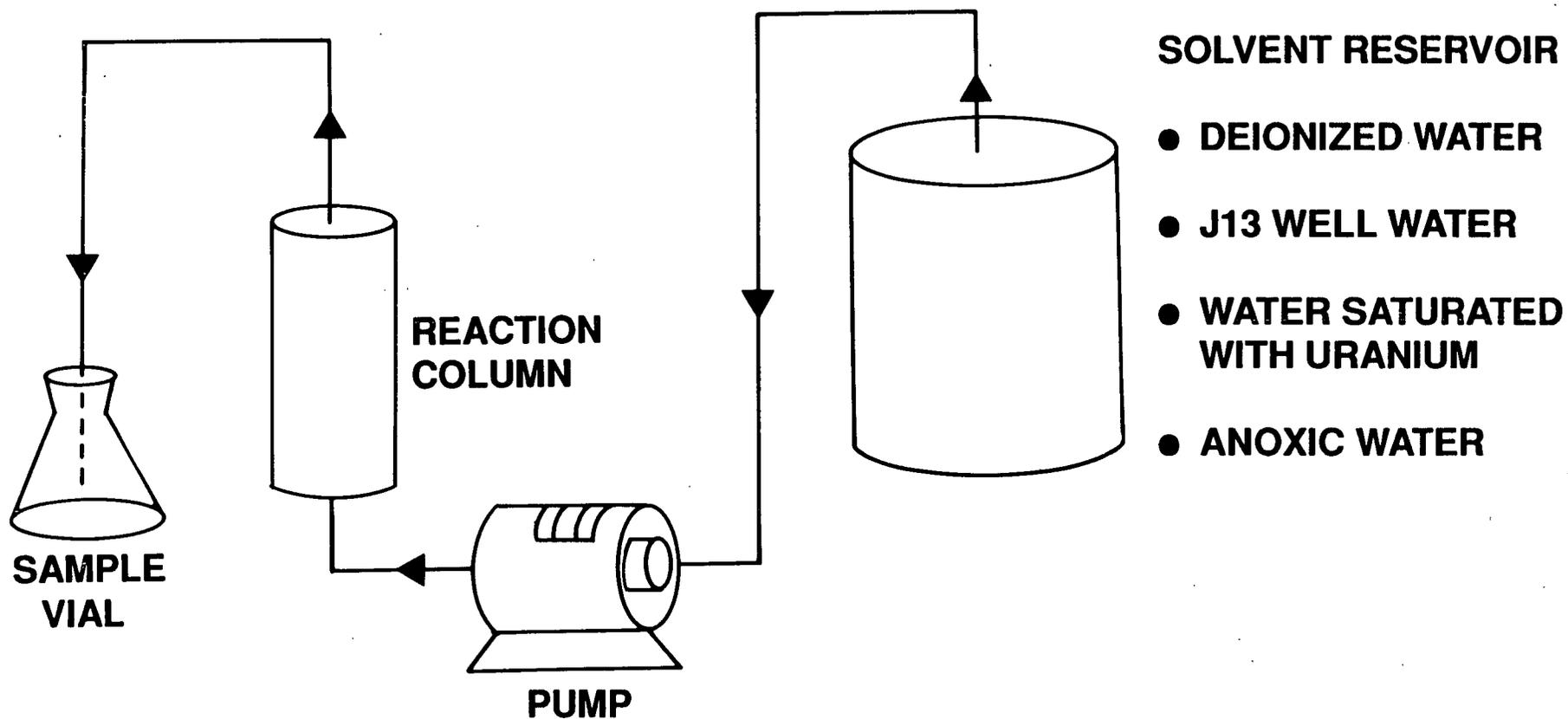
DESCRIPTION OF EXPERIMENT

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 UO₂ MATRIX AND CONTAINED RADIO-NUCLIDES
- MEASURE DISSOLUTION RATE OF UO₂ MATRIX AND CONTAINED RADIONUCLIDES

CONGRUENT DISSOLUTION APPARATUS



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:

$$\frac{\bar{X} - \mu}{s/\sqrt{n}} = t, \text{ COMPARE TO } t_{\alpha}(n - 1)$$

\bar{X} - MEAN OF OBSERVED RATIOS
 μ - TRUE RATIO VALUE
 n - NUMBER OF TESTS
 α - CONFIDENCE LEVEL

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

$$t = 2.17 < t_{\alpha}(2)$$

IF MEAN RATIO ≤ 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 $N = 5, s = .80, \bar{X} = 1.0$
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

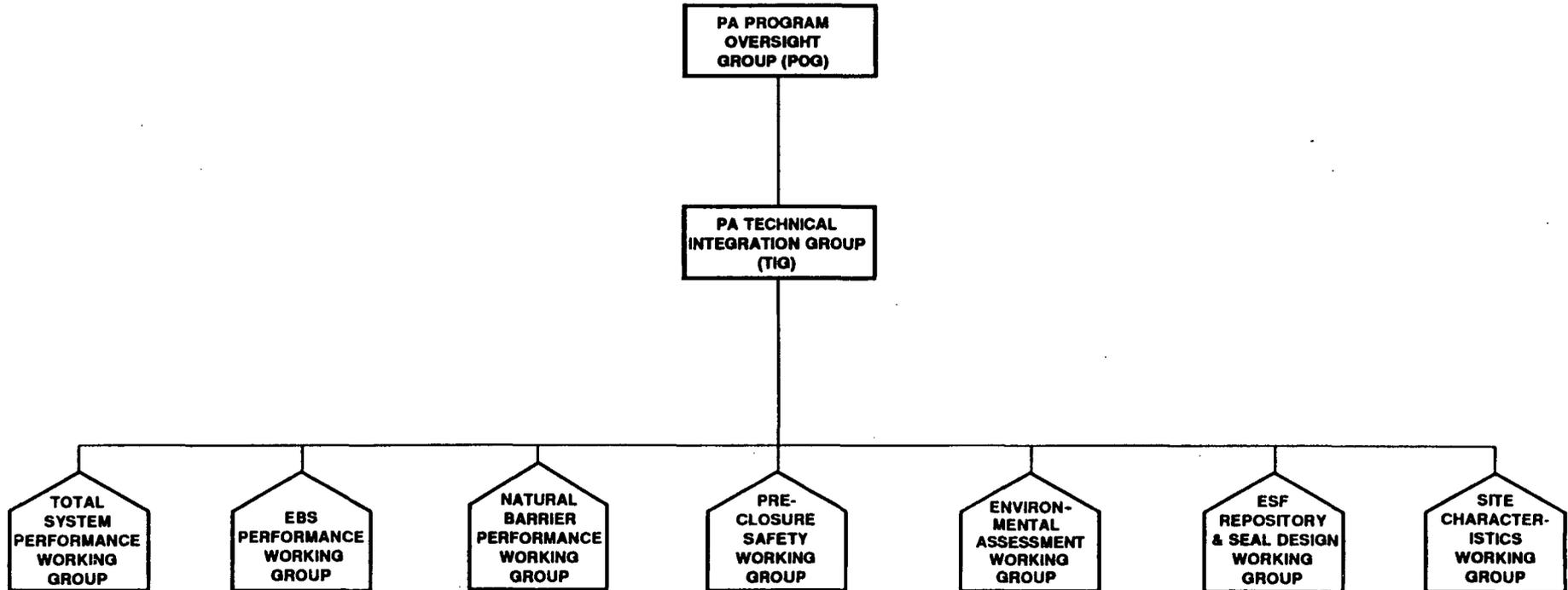
● DYNAMIC DISSOLUTION EXPERIMENTS

- 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.