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

PRESENTATION TO THE NUCLEAR WASTE TECHNICAL REVIEW BOARD

SUBJECT: HIGH-LEVEL WASTE GLASS CHARACTERIZATION OVERVIEW

PRESENTER: DR. HENRY SHAW

PRESENTER'S TITLE AND ORGANIZATION: GEOCHEMIST
LAWRENCE LIVERMORE NATIONAL LABORATORY
LIVERMORE, CALIFORNIA

PRESENTER'S TELEPHONE NUMBER: (415) 423-4645

AUGUST 28-29, 1990

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STATEMENT OF GLASS TASK GOALS

- THE PURPOSE OF THE GLASS WASTE FORM TASK IS TO DEVELOP THE DATA AND MODELS NEEDED TO PREDICT THE BEHAVIOR OF THE GLASS WASTE FORMS IN A YUCCA MOUNTAIN REPOSITORY OVER THE PERIOD OF REGULATORY CONCERN

- THIS INFORMATION IS USED IN PERFORMANCE ASSESSMENTS TO CALCULATE THE RELEASE OF RADIONUCLIDES FROM BREACHED GLASS WASTE CONTAINERS OVER TIME

- SUCH ASSESSMENTS ARE REQUIRED
  - TO DEMONSTRATE COMPLIANCE WITH THE CONTAINMENT AND CONTROLLED RELEASE REQUIREMENTS OF 10 CFR 60.113
  - AS THE BASIS OF THE GLASS SOURCE TERM IN ASSESSING COMPLIANCE WITH THE CUMULATIVE RELEASE LIMITS OF 40 CFR 191.13

THE PATH TOWARD ACHIEVING THE GOALS

- ACQUIRE SITE AND OTHER WASTE PACKAGE CHARACTERISTICS DATA FROM OTHER PROJECT TASKS
- ACQUIRE WASTE FORM CHARACTERISTICS DATA FROM WASTE PRODUCERS (e.g., PHYSICAL DIMENSIONS, RADIONUCLIDE INVENTORY, CHEMICAL COMPOSITION)
- CONDUCT SITE-RELEVANT EXPERIMENTS TO IDENTIFY GLASS DEGRADATION MECHANISMS, MATERIALS INTERACTIONS, POST-ALTERATION RADIONUCLIDE DISTRIBUTIONS, ETC.
- DEVELOP "MECHANISTIC" CHEMICAL/PHYSICAL MODELS THAT DESCRIBE IMPORTANT PROCESSES

THE PATH TOWARD ACHIEVING THE GOALS

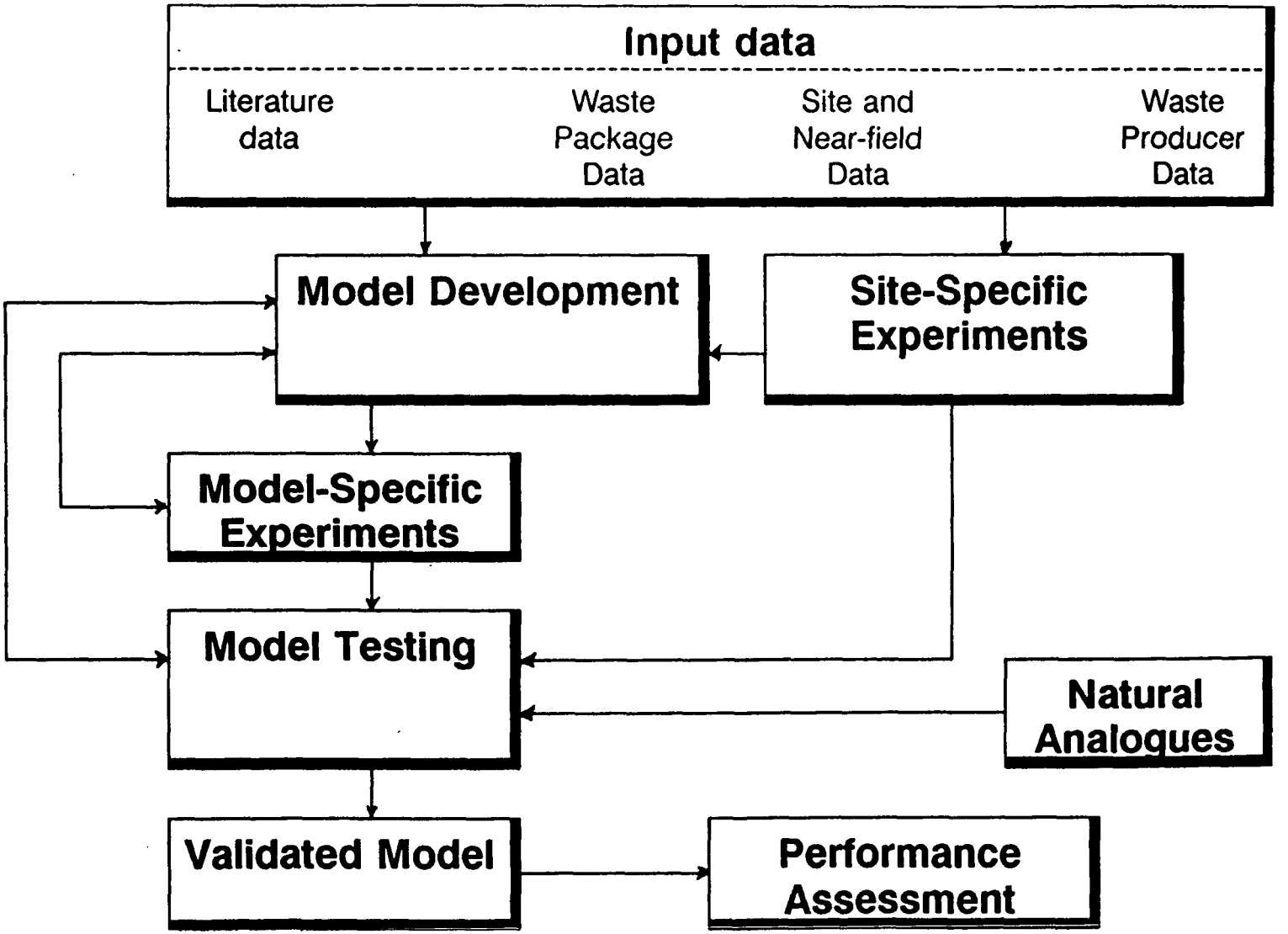
(CONTINUED)

- CONDUCT MODEL-SPECIFIC EXPERIMENTS TO PROVIDE DATA FOR USE IN MODELS AND TO TEST POSTULATED MECHANISMS AND PROCESSES IN ISOLATION

- COMPARE MODEL PREDICTIONS WITH "LONG-TERM", SITE-RELEVANT TEST AND NATURAL ANALOGUE DATA

- IDENTIFY MISSING DATA AND/OR MODEL DEFICIENCIES AND ITERATE ON THE ABOVE STEPS UNTIL CONVERGENCE IS OBTAINED

GLASS TASK INFORMATION FLOW



GLASS MODELING APPROACH

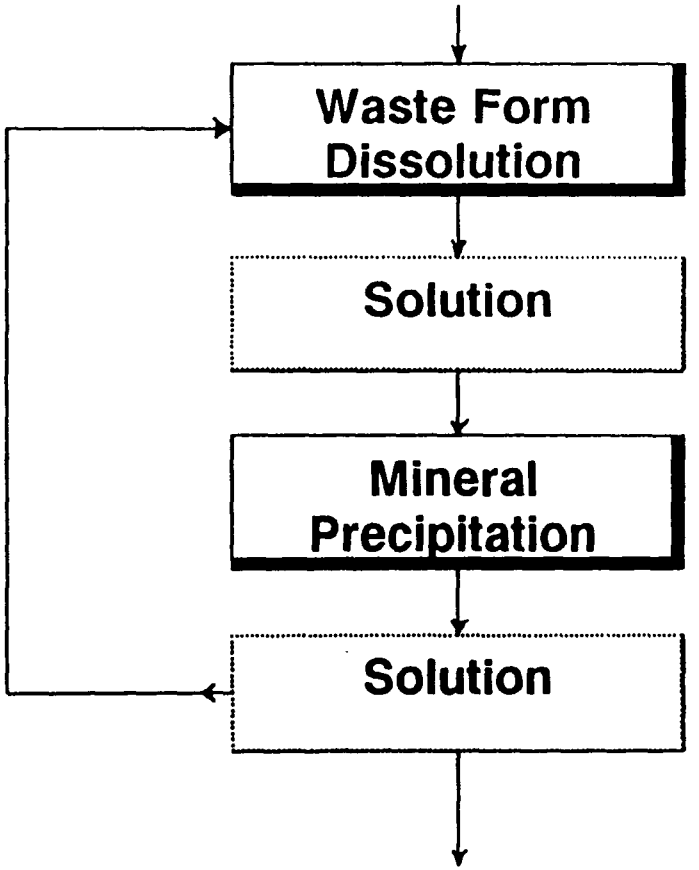
- CURRENT EFFORTS CENTER ON UNDERSTANDING CONTROLS ON THE RATES AND NATURE OF THE CHEMICAL REACTIONS OCCURRING AT THE GLASS-WATER INTERFACE

- PRESENT EVIDENCE SUPPORTS THE REACTION OF A PARTIALLY ALTERED "GEL LAYER" AS THE RATE-LIMITING STEP

- A KINETIC MODEL INCORPORATING THIS IDEA HAS BEEN DEVELOPED. ITS PREDICTIONS ARE BEING TESTED AGAINST THE RESULTS OF VARIOUS EXPERIMENTS

- THE CALCULATIONAL FRAMEWORK USED CAN BE EXTENDED TO INCLUDE OTHER IMPORTANT PROCESSES AS THEY ARE IDENTIFIED AND ABSTRACTED INTO MODELS

GLASS DISSOLUTION MODELING APPROACH

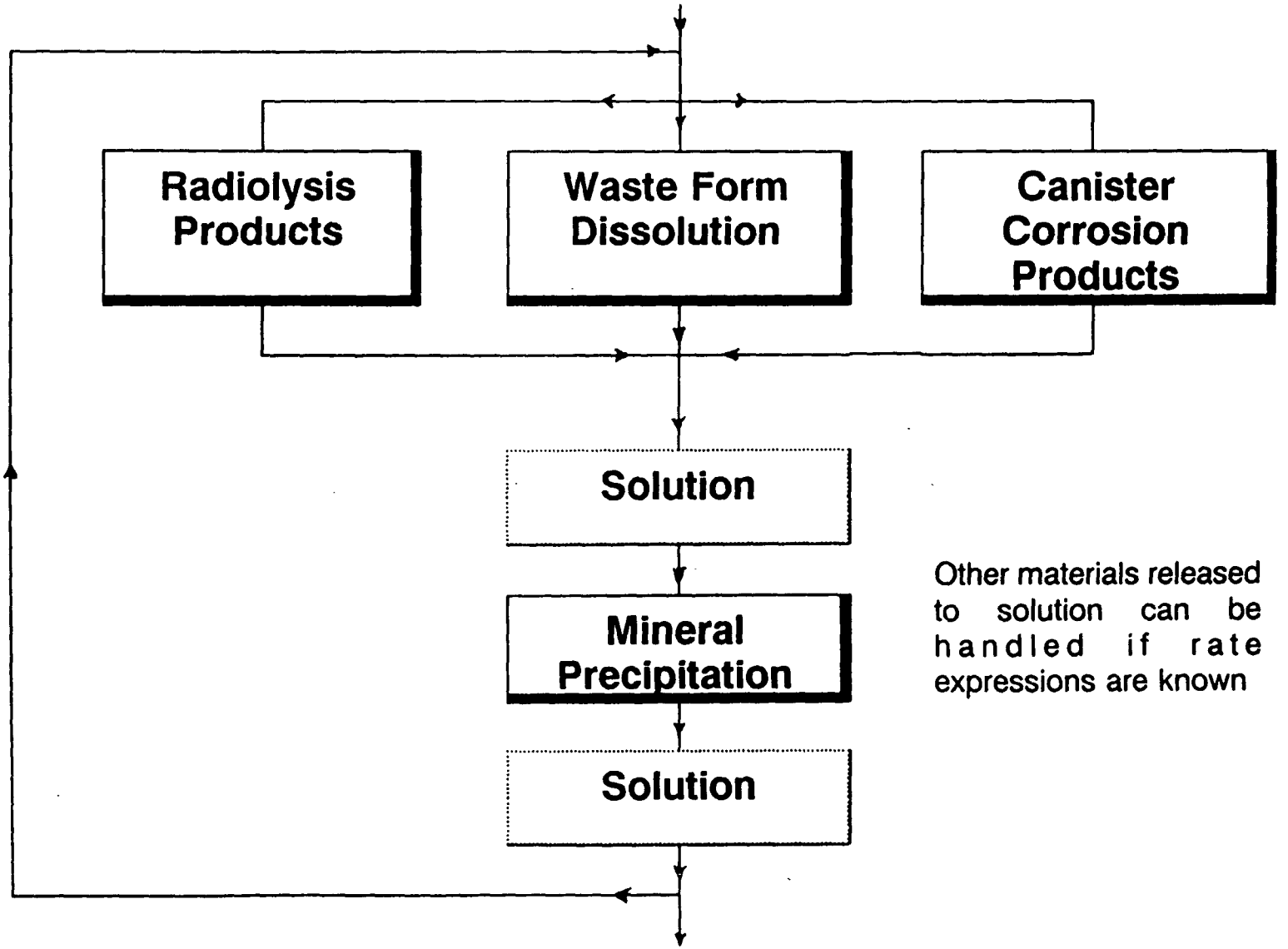


Dissolution rate depends on temperature, glass composition, and solution composition.

EQ3/6 code is used to determine mineral saturation. Secondary phases can either remain in the system or be isolated.

New solution composition is fed back to dissolution rate model and the rate is adjusted.

THIS APPROACH CAN BE EXTENDED TO INCLUDE OTHER PROCESSES



Other materials released to solution can be handled if rate expressions are known

PURPOSE OF MODEL-SPECIFIC EXPERIMENTS

MODEL-SPECIFIC EXPERIMENTS ARE USED TO

- DETERMINE KEY PARAMETERS NEEDED BY THE MATHEMATICAL MODELS
- ISOLATE SPECIFIC PROCESSES SO THEY CAN BE STUDIED IN THE ABSENCE OF CONFOUNDING EFFECTS
- DETERMINE THE FUNCTIONAL DEPENDENCE OF RATES ON THE VALUE OF INDIVIDUAL PARAMETERS (e.g., pH) WHILE OTHERS ARE HELD CONSTANT

PURPOSE OF SITE-SPECIFIC EXPERIMENTS

- SITE-SPECIFIC EXPERIMENTS ARE NOT ADEQUATE AS A BASIS FOR LONG-TERM PREDICTIONS

SITE-SPECIFIC EXPERIMENTS DO

- PROVIDE LABORATORY-SCALE SIMULATION OF RELEVANT PROCESSES

- PROVIDE PHENOMENOLOGY OF GLASS ALTERATION PROCESS
  - TYPES AND QUANTITIES OF SECONDARY PHASES
  - COMPOSITIONS AND TEXTURES OF ALTERATION LAYERS
  - INTERACTIONS BETWEEN GLASS AND WASTE PACKAGE MATERIALS (e.g., POUR CANISTER)
  - OVERALL RELEASE RATE OF ELEMENTS TO SOLUTION

- PROVIDE AN INDEPENDENT DATABASE AGAINST WHICH TO TEST MODEL PREDICTIONS

NWTRB MEETING - LLNL-YMP HLW GLASS CHARACTERIZATION AGENDA

HLW GLASS CHARACTERIZATION OVERVIEW	DR. HENRY SHAW (GEOCHEMIST, LLNL)
MODELING OF GLASS DISSOLUTION	DR. WILLIAM BOURCIER, (GEOCHEMIST, GLASS TASK LEADER, LLNL)
EXPERIMENTAL BASES FOR GLASS MODELING	DR. KEVIN KNAUSS, (GEOCHEMIST, LLNL)
INTEGRATED GLASS ALTERATION TESTS	DR. JOHN BATES, (CHEMIST, ARGONNE NATIONAL LABORATORY)