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

PRESENTATION TO THE NUCLEAR WASTE TECHNICAL REVIEW BOARD

SUBJECT: PASS PROGRAM

PRESENTER: DR. M. J. APTED

PRESENTER'S TITLE AND ORGANIZATION:
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PASS PROGRAM
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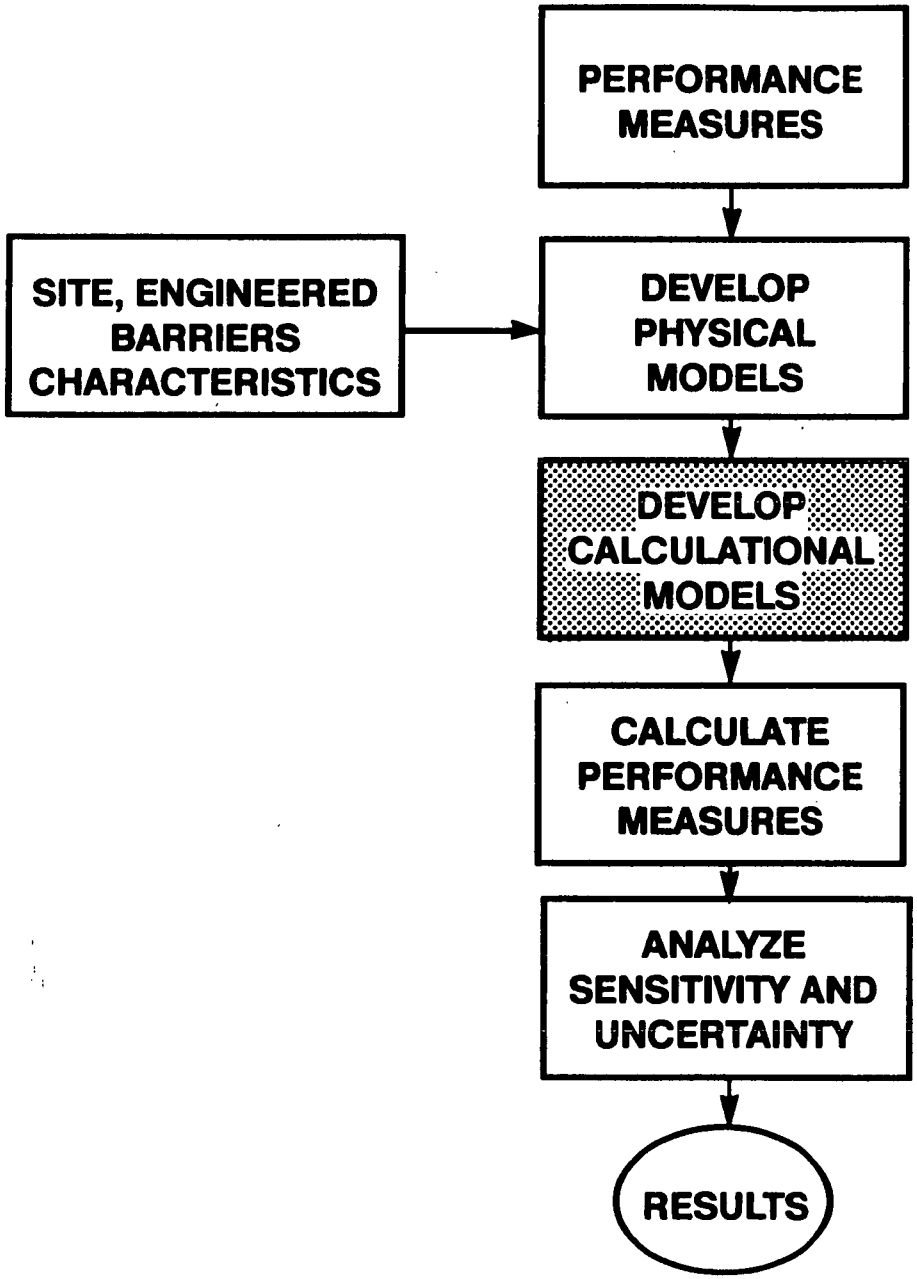
MAY 16-17, 1989

SCOPE OF PRESENTATION

- STRUCTURE OF AREST CODE
- TYPICAL RESULTS
- BENCHMARKING
- FUTURE ACTIVITIES

PERFORMANCE ASSESSMENT PROCESS



ANALYTIC REPOSITORY SOURCE-TERM (AREST) CODE

- INTEGRATES PROCESS SUBMODELS
  - NEAR-FIELD ENVIRONMENT
  - CONTAINMENT
  - RELEASE
- CALCULATES ENGINEERED BARRIER SYSTEM (EBS) PERFORMANCE
- CAPABLE OF PROBABILISTIC ANALYSES

APPROACH TO AREST SUBSYSTEM MODELING

DIVIDE THE ASSESSMENT INTO FOUR SEPARATE PARTS:

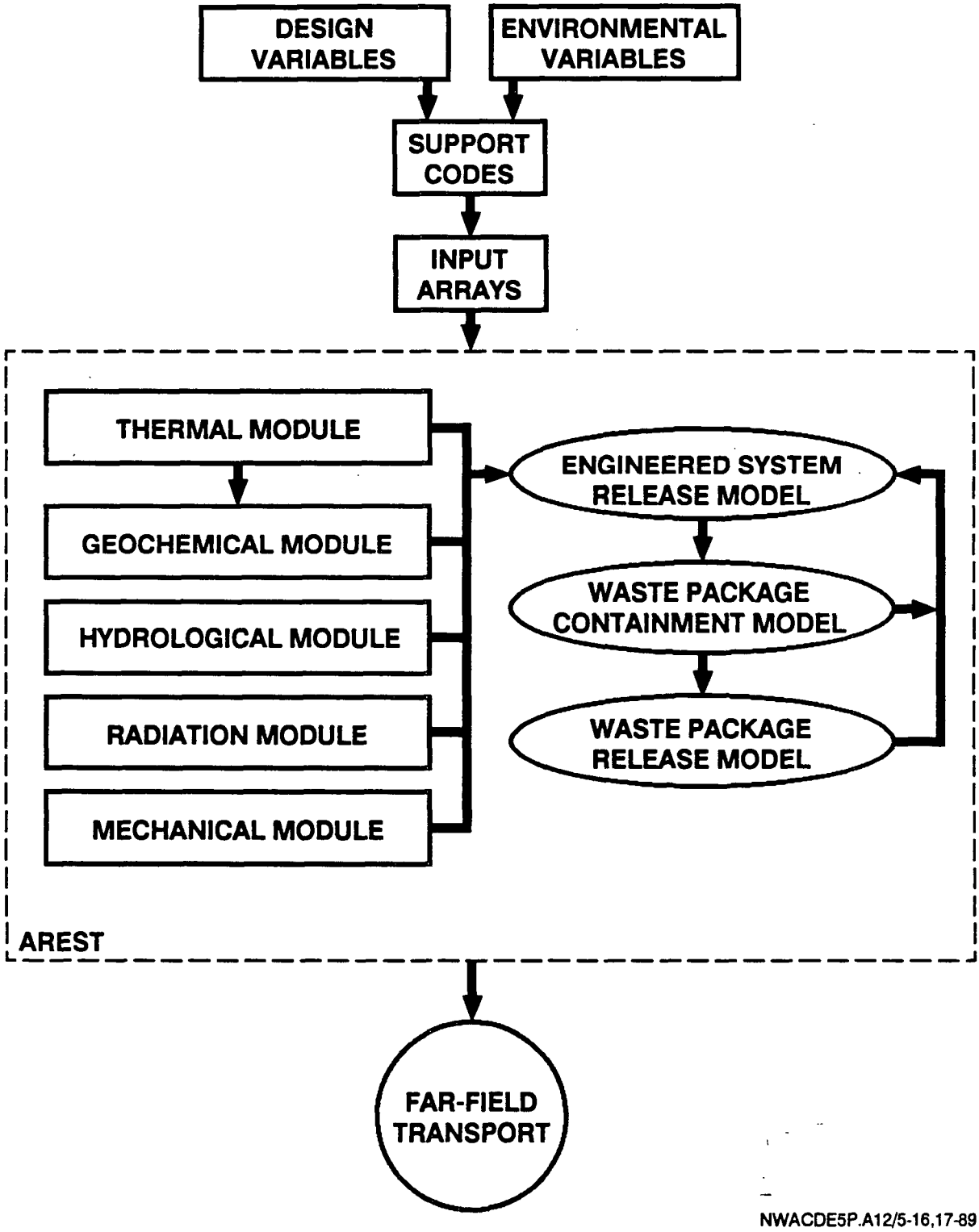
1) **OBTAIN INPUT DATA, INCLUDING WASTE PACKAGE DESIGN, REPOSITORY LOGISTICS, AND SITE CHARACTERIZATION**

2) **USE DETAILED-THERMAL-MECHANICAL-HYDROLOGICAL CODES ("SUPPORT CODES") TO ANALYZE AND TABULATE THE EVOLUTION OF THE NEAR-FIELD ENVIRONMENT OVER TIME AND SPACE**

3) **DEVELOP MODULAR, MATERIAL-SPECIFIC MODELS AFFECTING THE CONTAINMENT, RELEASE, AND MASS TRANSFER INTO THE HOST ROCK OF RADIONUCLIDES FROM INDIVIDUAL WASTE PACKAGES**

4) **INTEGRATE THE BEHAVIOR OF INDIVIDUAL WASTE PACKAGES TO PROVIDE A PROBABILISTIC ASSESSMENT OF THE OVERALL CONTAINMENT AND RELEASE PERFORMANCE OF THE EBS**

SUPPORT CODE/AREST MODEL INTERFACE



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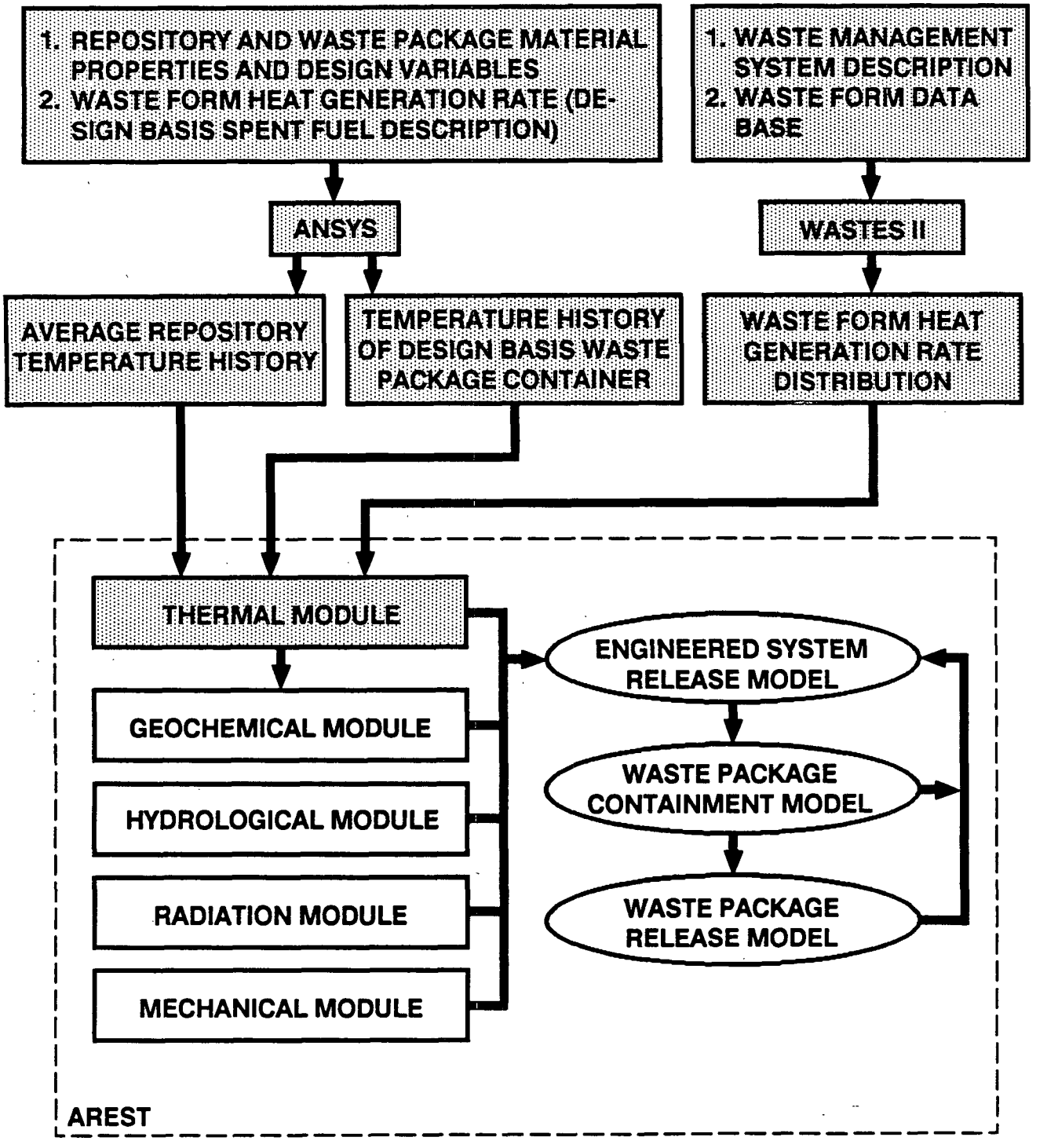
TECHNIQUES FOR BUILDING A SUBSYSTEM MODEL

- MODULAR STRUCTURE
- SIMPLIFY DETAILED PROCESS MODELS
  - ALGORITHMS
  - TABULATIONS
- SELECT TEMPERATURE AS PRIME PARAMETER
- EVALUATE IMPORTANCE OF COUPLED PROCESSES
- SIMPLIFY GEOMETRY

EXAMPLE 1: DERIVATION OF AREST THERMAL MODULE



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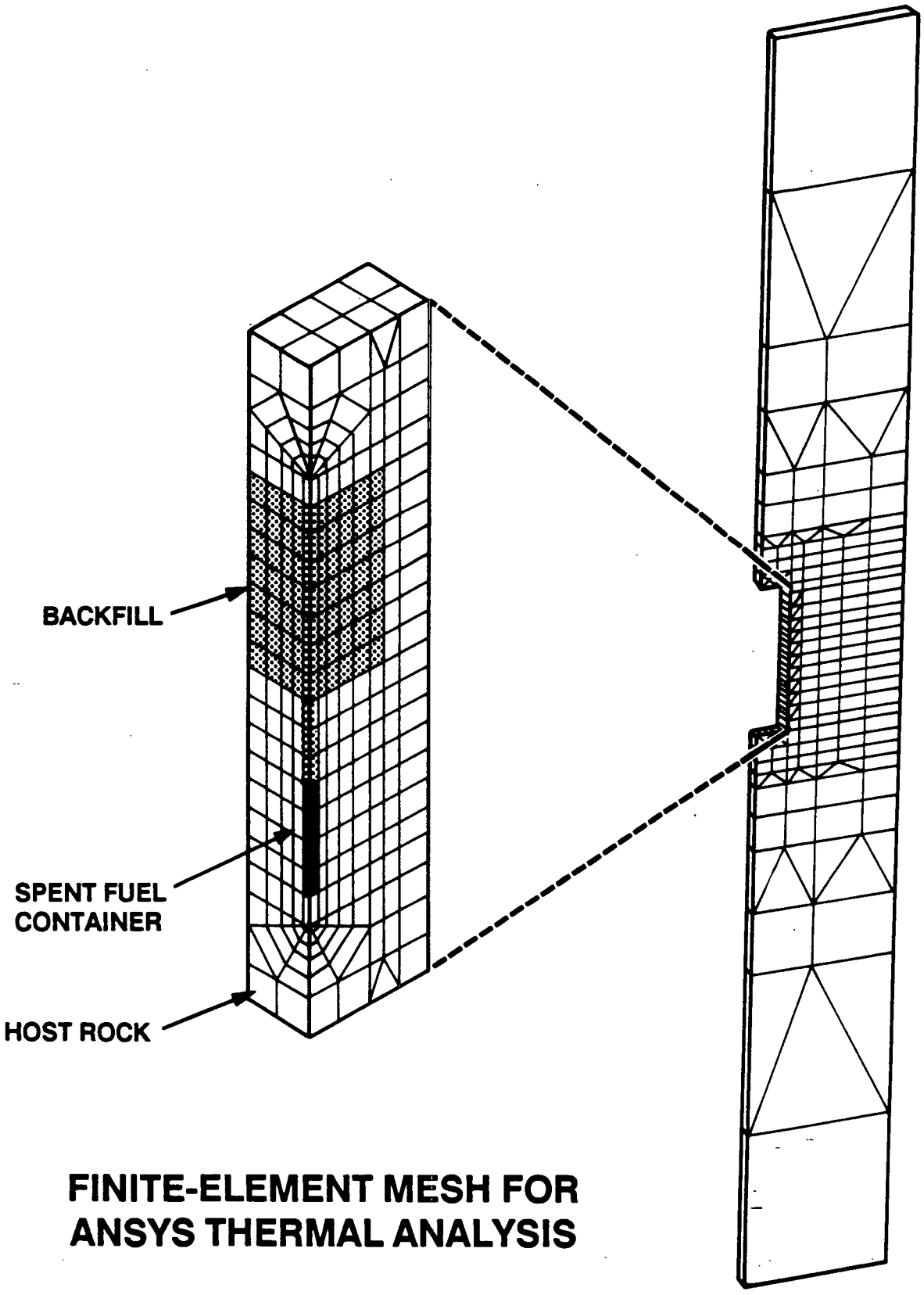
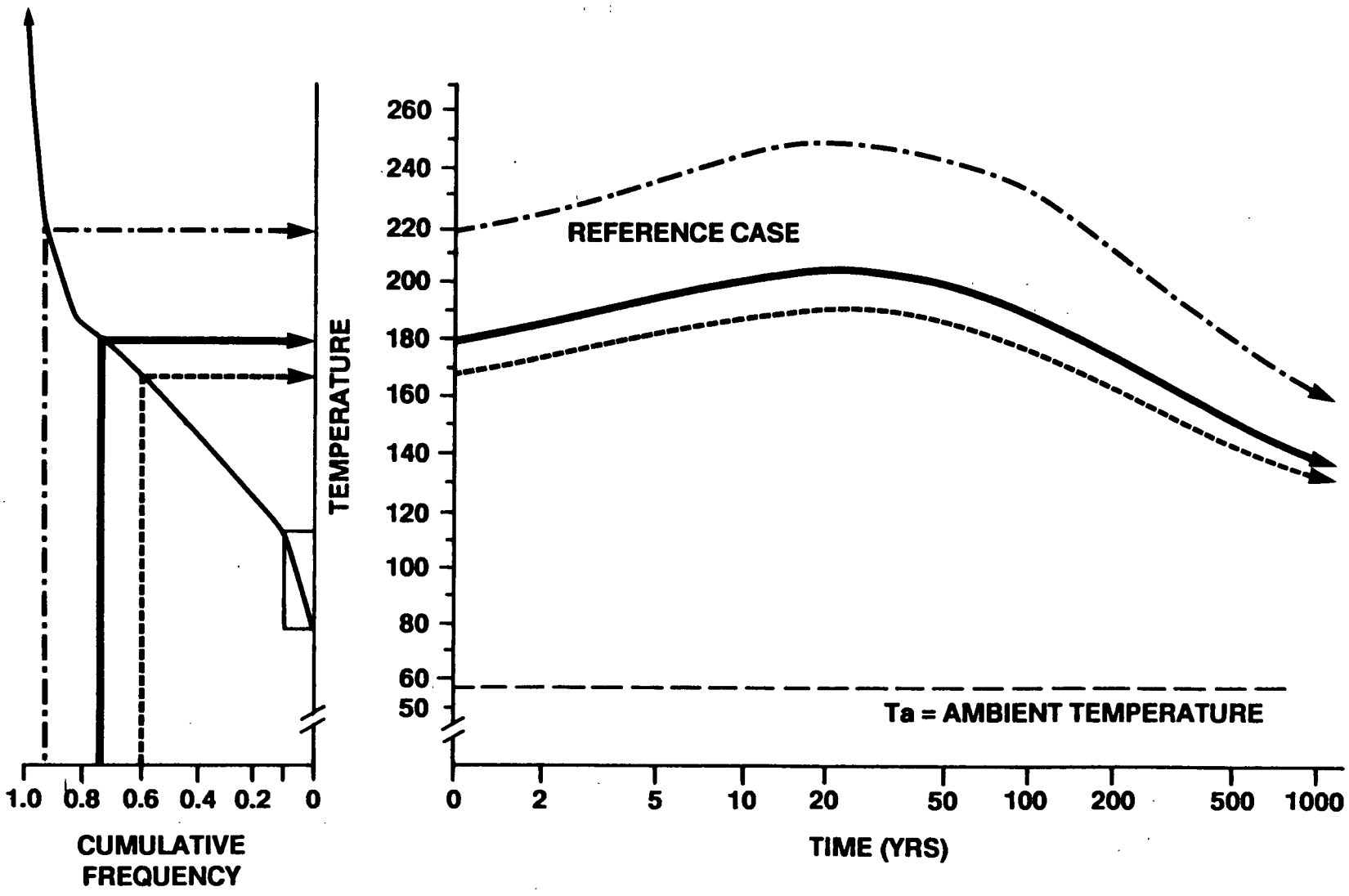
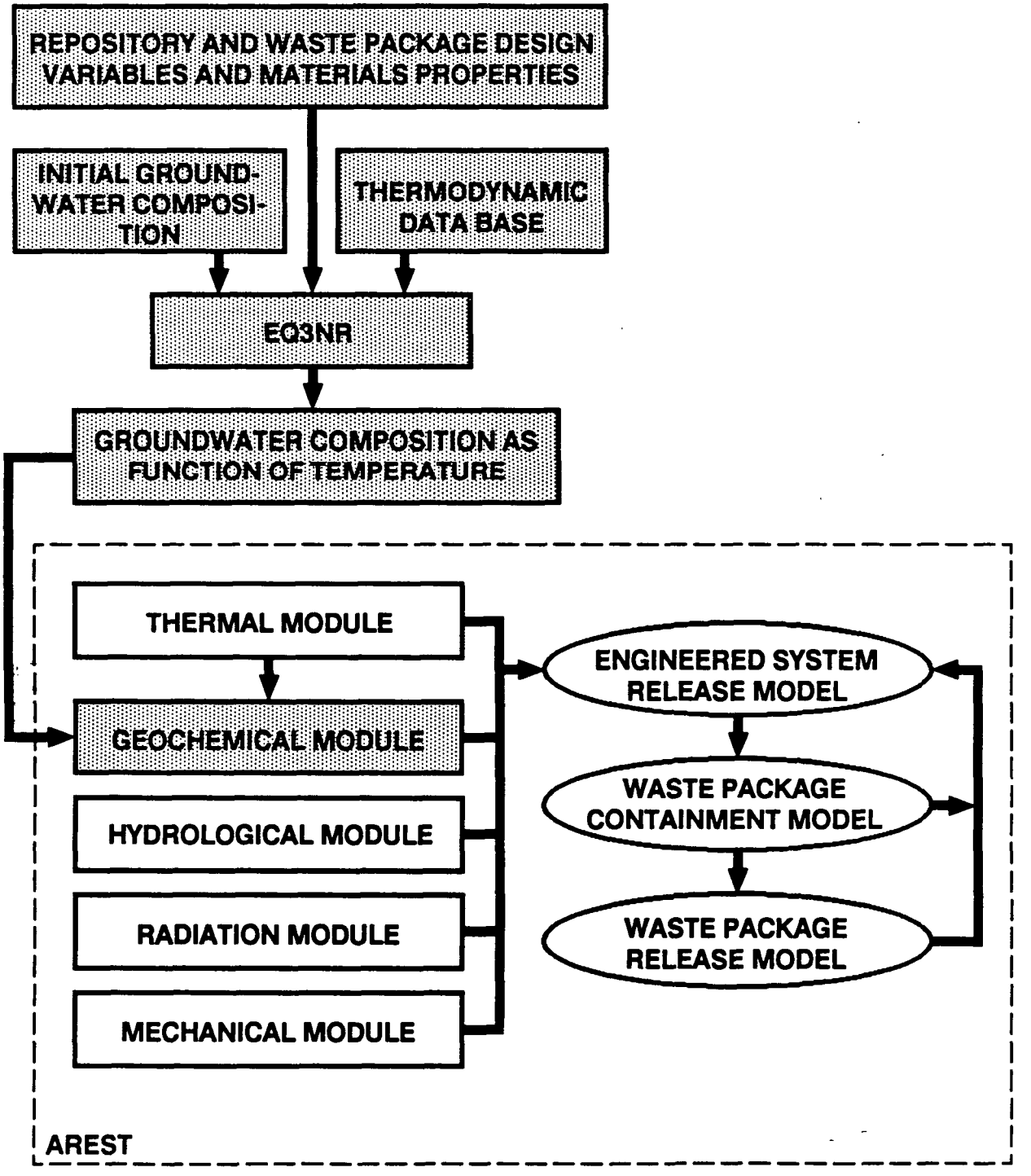


FINITE-ELEMENT MESH FOR ANSYS THERMAL ANALYSIS



DERIVATION OF TEMPERATURE PROFILES

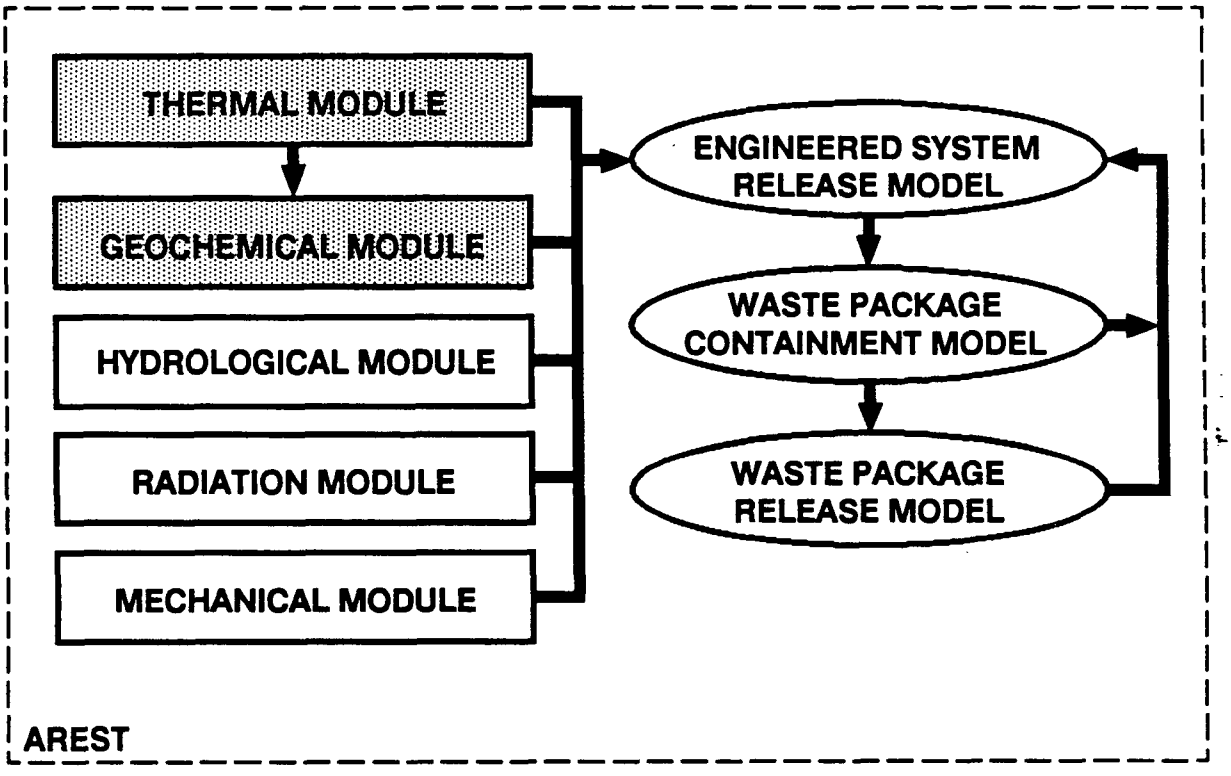
EXAMPLE 2: DERIVATION OF AREST GEOCHEMICAL MODULE



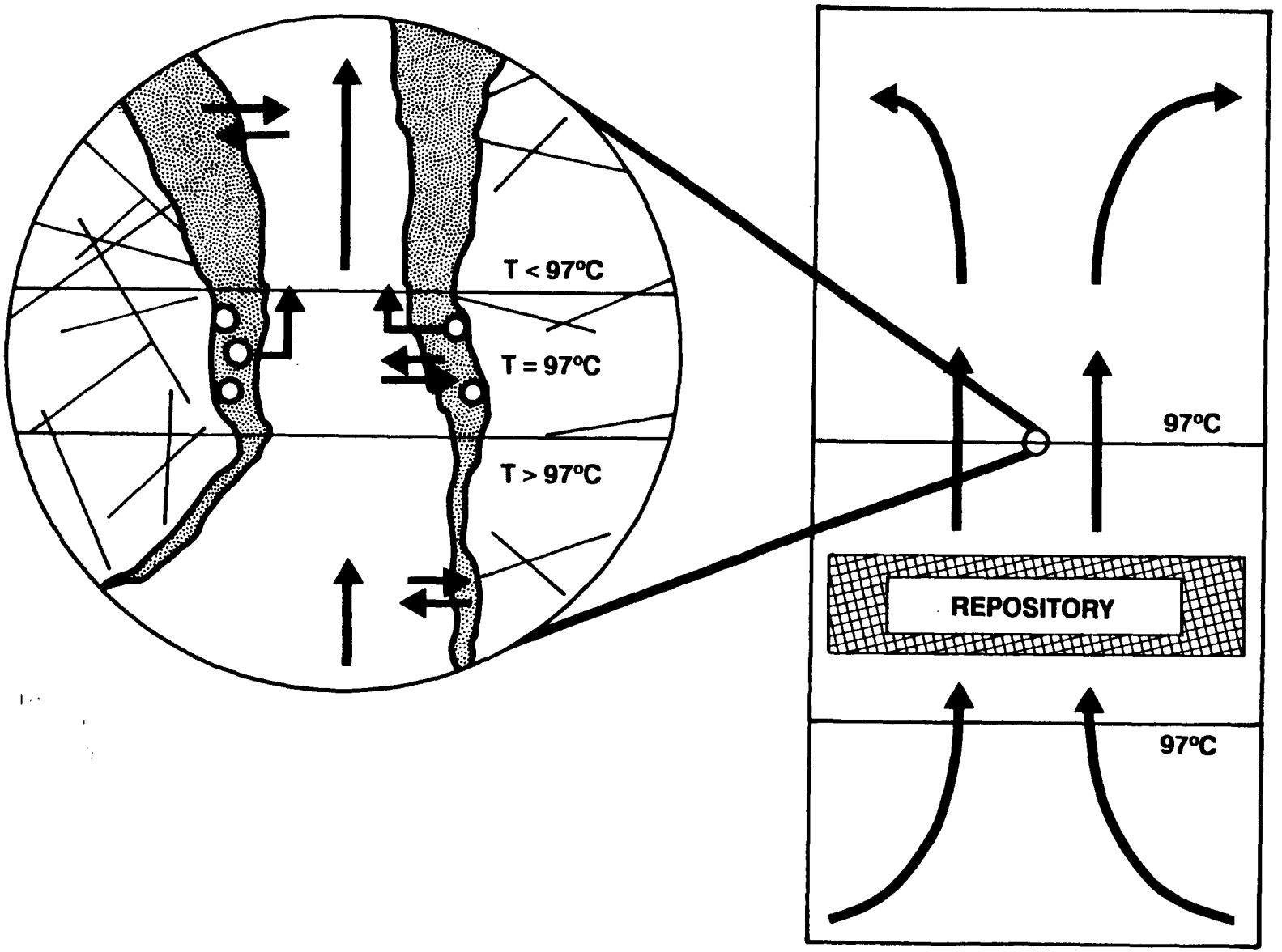
EXAMPLE 2: TABULATED GROUNDWATER COMPOSITION

SPECIES	CONCENTRATION (mol/kg)		
T (°C)	55	60	65
pH (T)	7.45	7.42	7.40
Eh (V)	-0.345	-0.346	-0.347
ρ	1.023	1.020	1.019
Na^+	0.1398D-01	0.1466D-01	0.1571D-01
Cl^-	0.1038D-01	0.1083D-01	0.1083D-01
$Al(OH)_4^-$	0.9431D-03	0.1617D-02	0.2661D-02
SiO_2 (aq)	0.1445D-02	0.1439D-02	0.1436D-02
HCO_3^-	0.1431D-02	0.1025D-02	0.1430D-02
F	0.1025D-02	0.1025D-02	0.1025D-02
$H_3SiO_4^-$	0.1071D-03	0.1123D-03	0.1154D-03
Ca_2	0.5102D-04	0.5089D-04	0.5078D-04
HS^-	0.4149D-04	0.4143D-04	0.4130D-04
H_2CO_3	0.1977D-04	0.2053D-04	0.2185D.04
CO_3^{2-}	0.1877D-04	0.1860D-04	0.1797D-04
OH^-	0.1084D-04	0.1366D-04	0.1669D-04
NaCl	0.1070D-04	0.1092D-04	0.1146D-04
NaF	0.2406D-05	0.2703D-05	0.3092D-05
$NaCO_3^-$	0.1783D-05	0.1899D-05	0.2006D-05
H_2S (aq)	0.1313D-05	0.1272D-05	0.1272D-05
$CaHCO_3$	0.9615D-06	0.9783D-06	0.9941D-06
$CaCO_3$	0.8683D-06	0.9057D-06	0.9150D-06
CaF^+	0.7761D-06	0.8480D-06	0.9232D-06
SO_4^{2-}	0.1775D-06	0.2713D-06	0.3997D-06

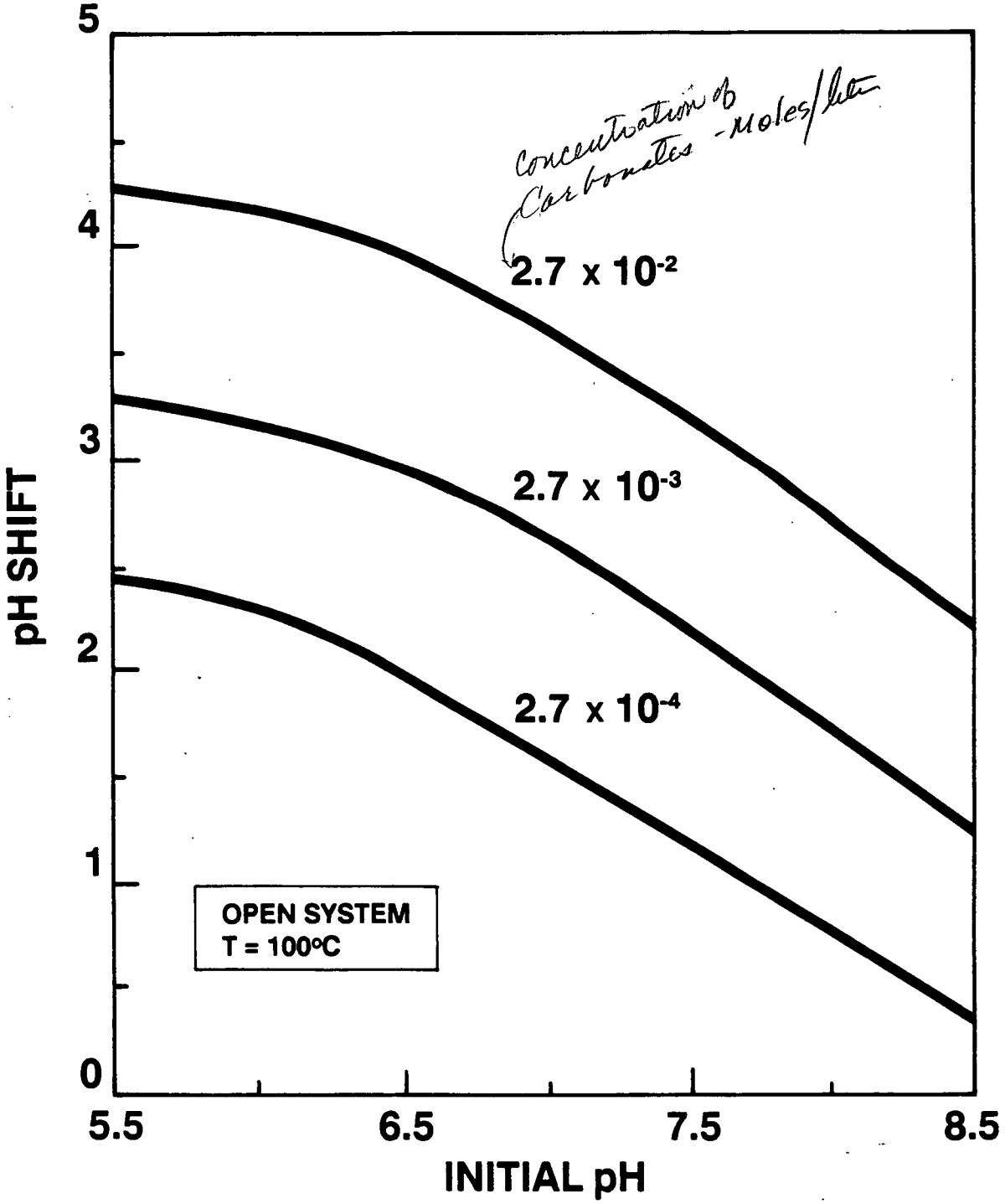
EXAMPLE 3: EVALUATE IMPORTANCE OF THERMAL-CHEMICAL COUPLING



SCHEMATIC OF BOILING FRONT AND ITS EFFECT ON GROUNDWATER CHEMISTRY



EFFECT OF BOILING ON pH OF GROUNDWATER CALCULATED WITH EQ 3/6



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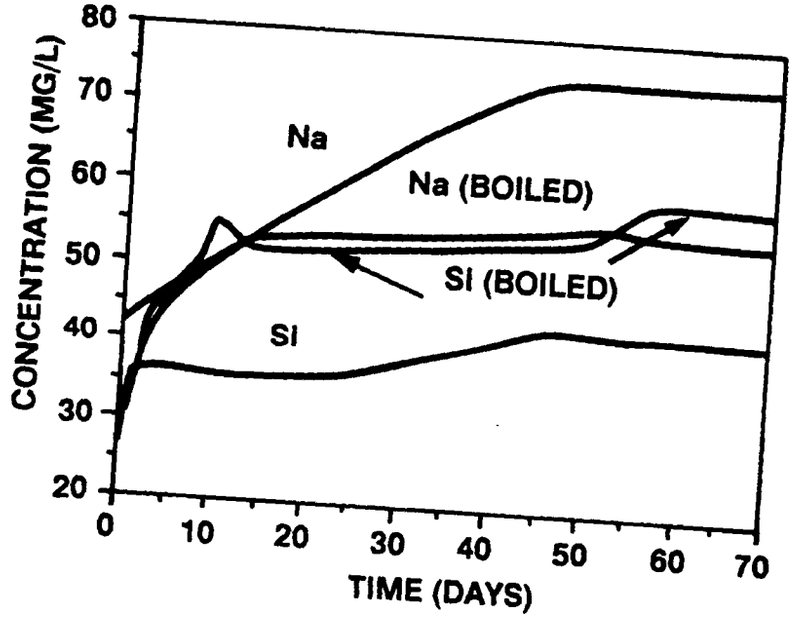
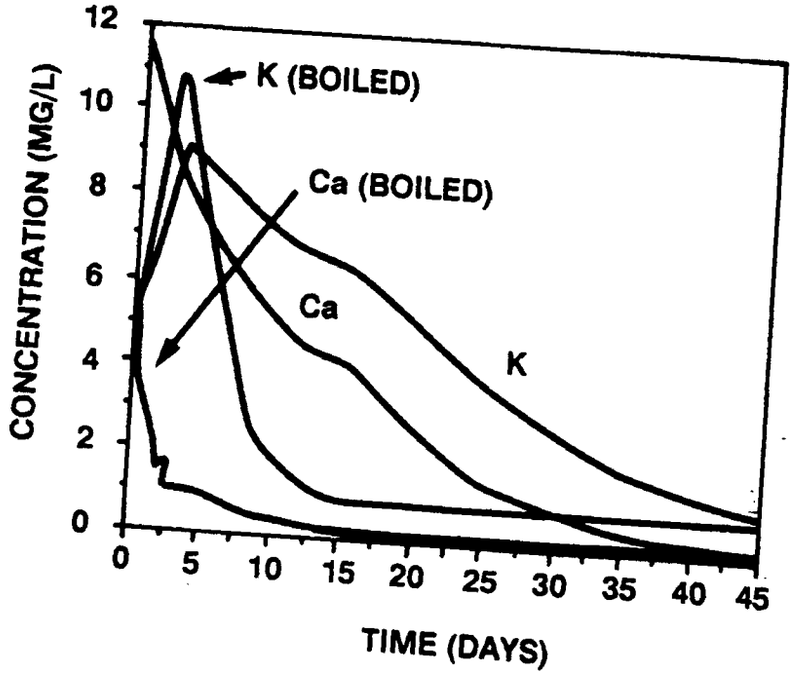
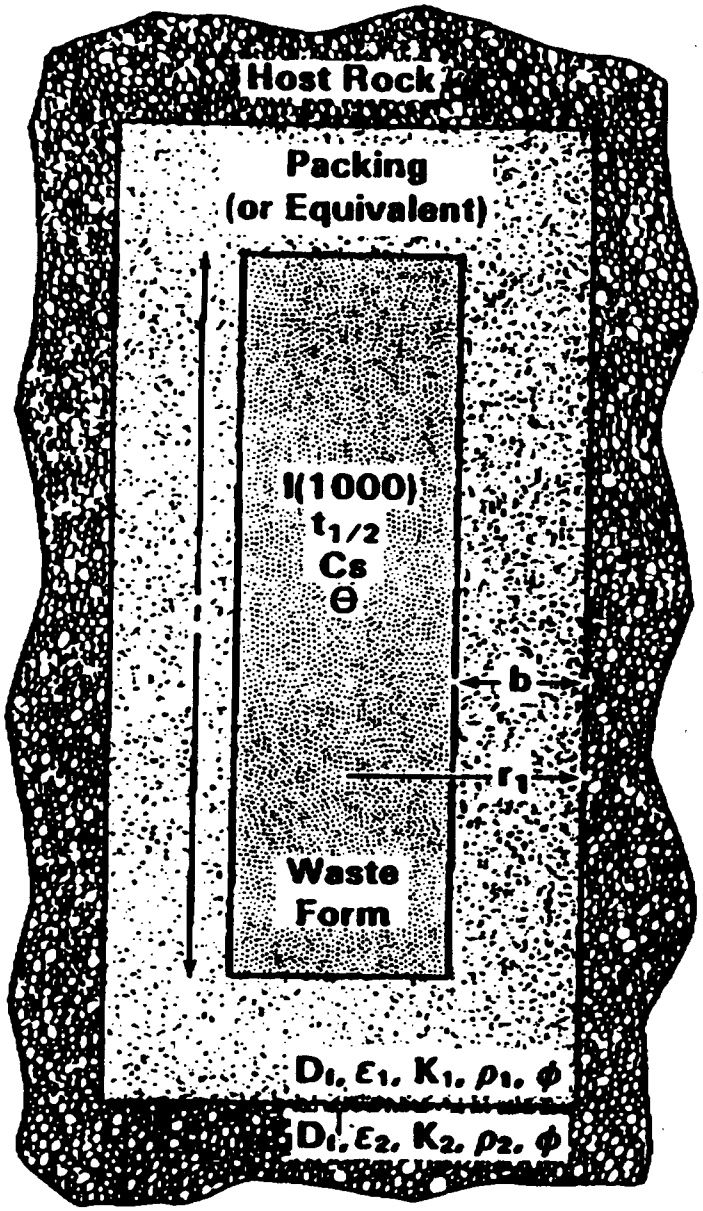
EFFECT OF BOILING ON GROUNDWATER COMPOSITION

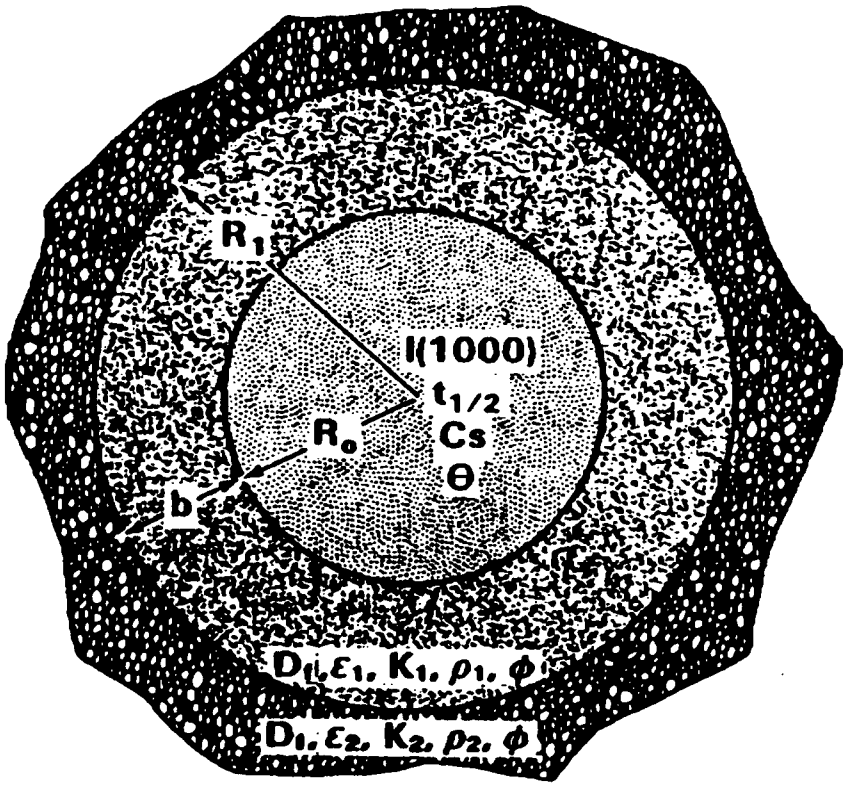




EXAMPLE 4: SIMPLIFY WASTE PACKAGE GEOMETRY

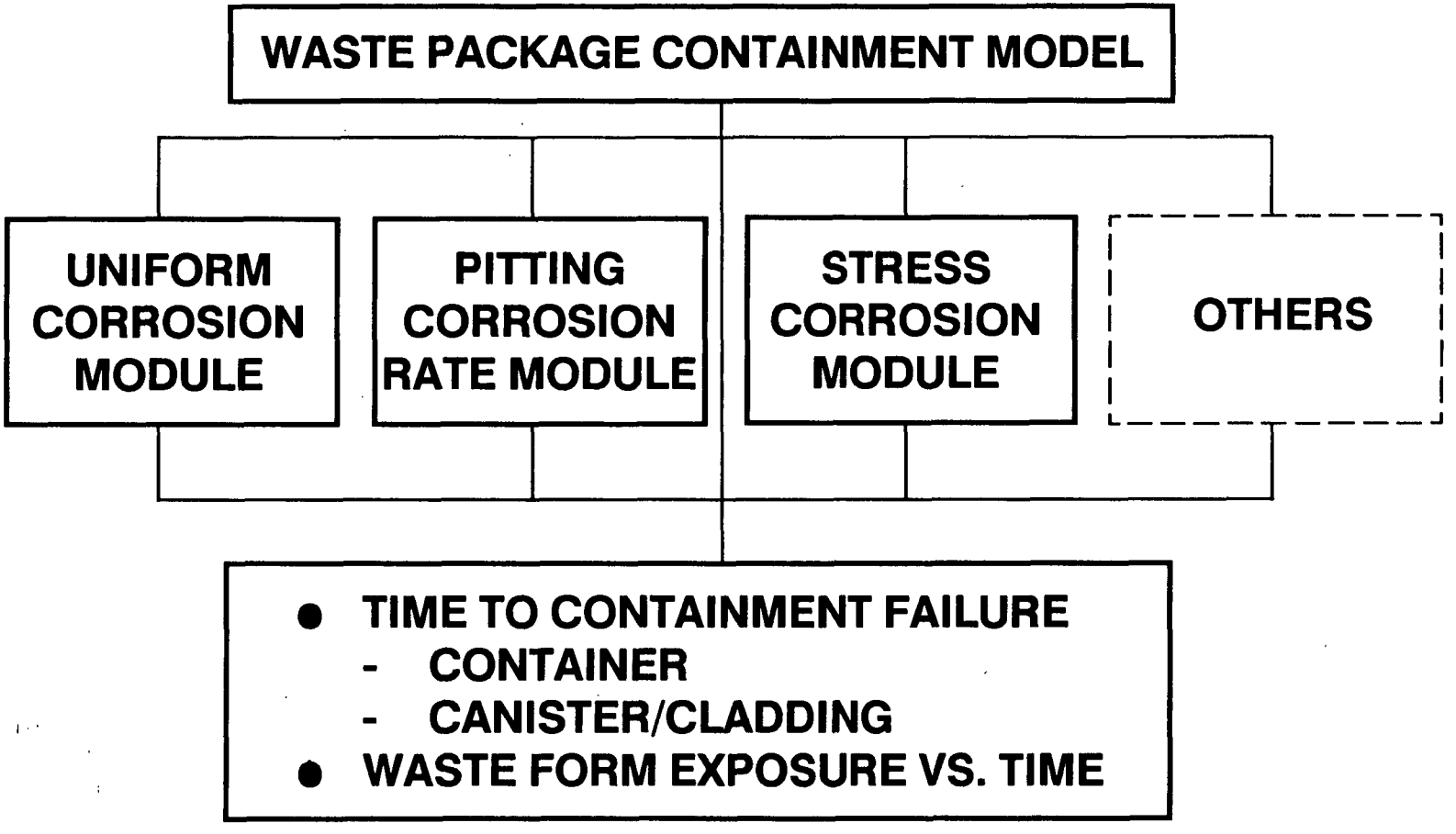


Actual Cylinder

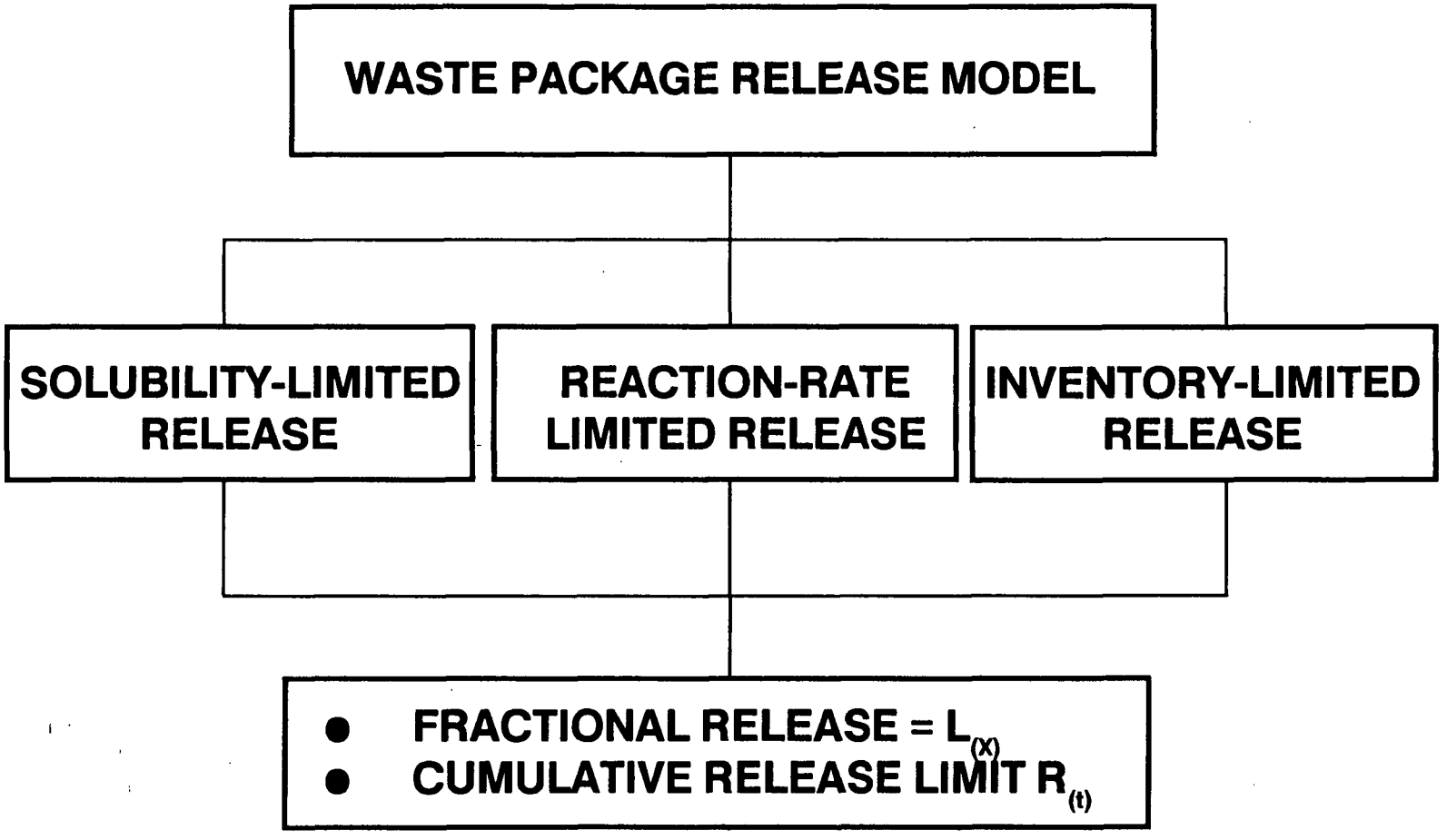


Equivalent Sphere

AREST: WASTE PACKAGE CONTAINMENT MODEL



AREST: WASTE PACKAGE RELEASE MODEL



SCOPE OF PRESENTATION

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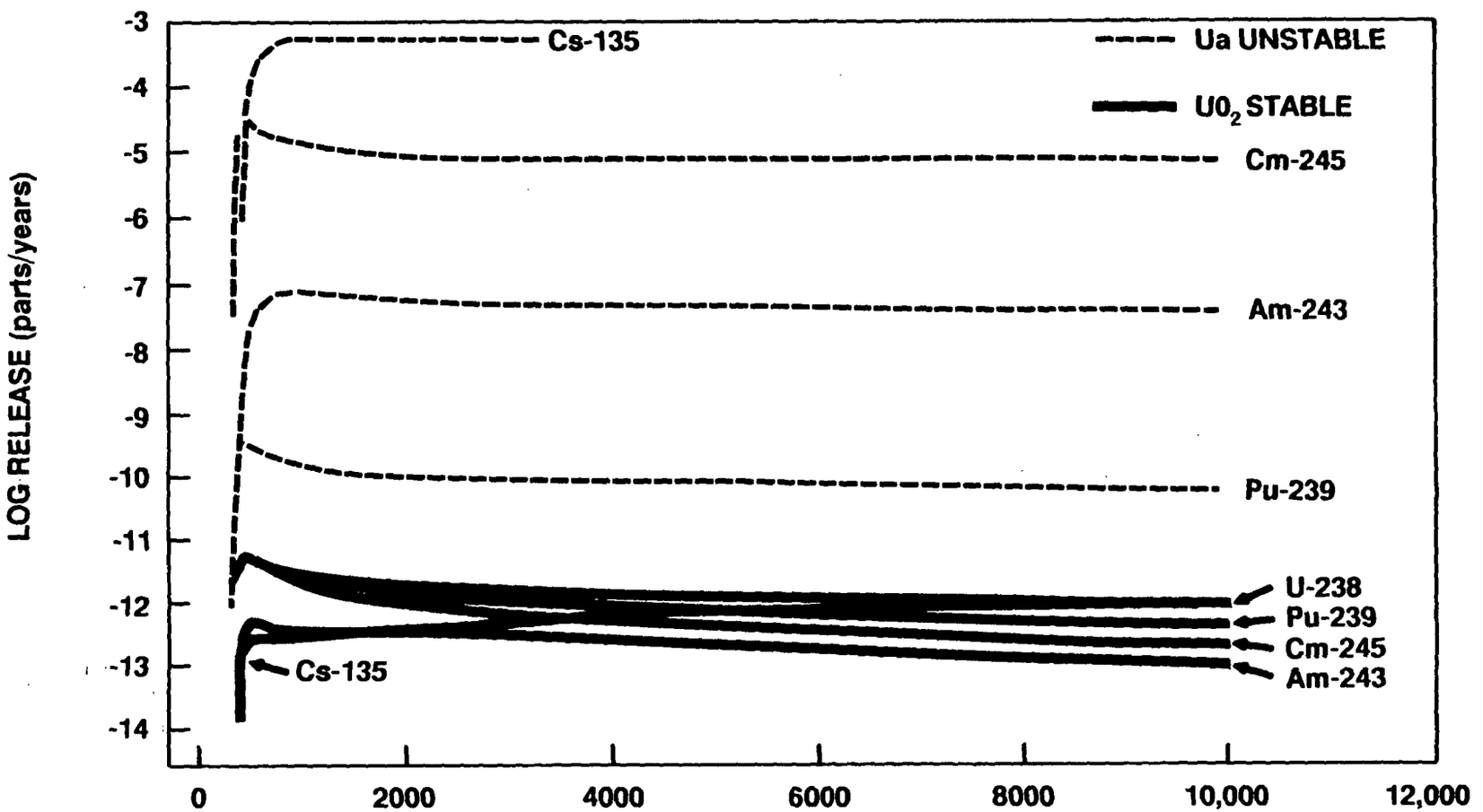
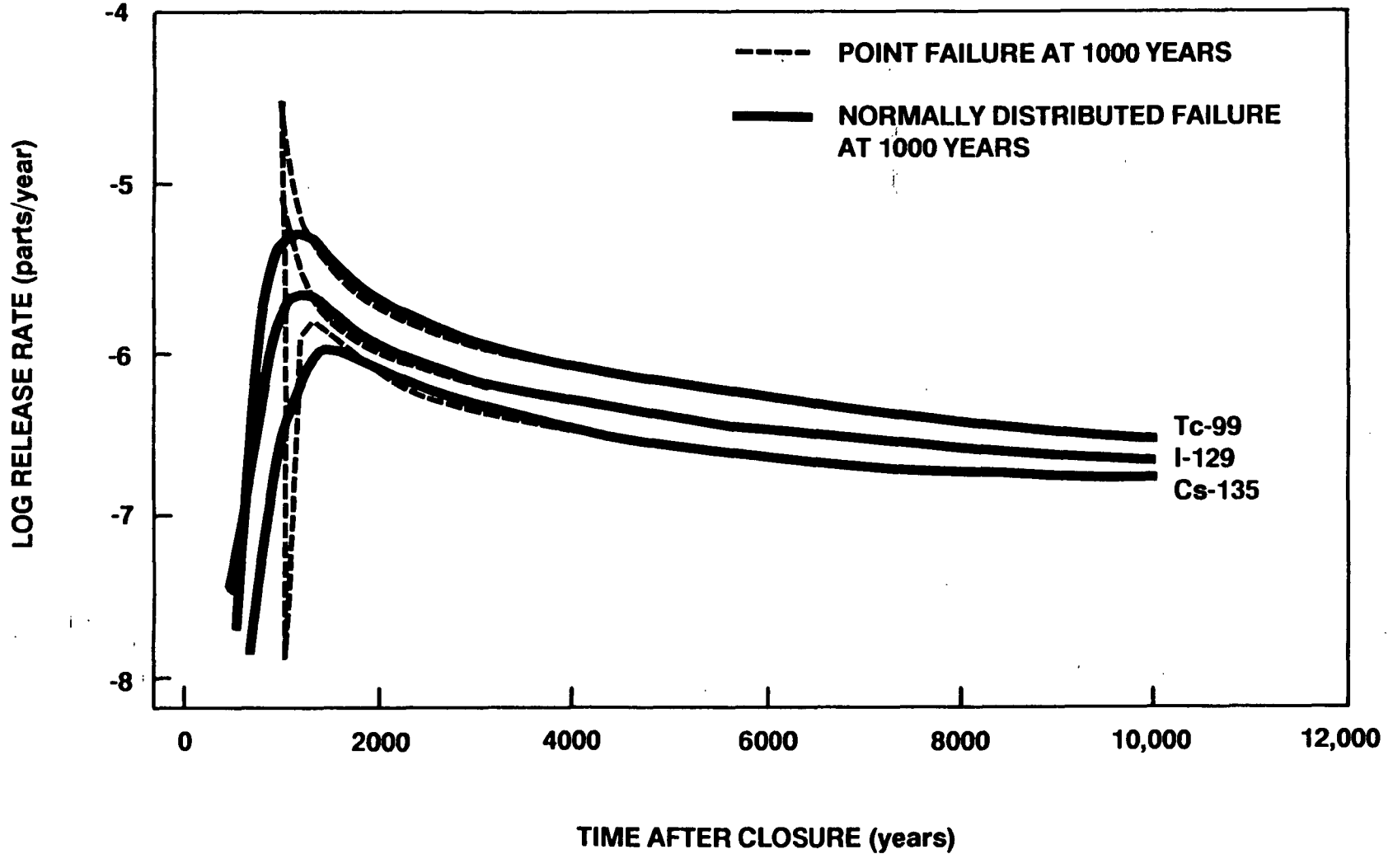
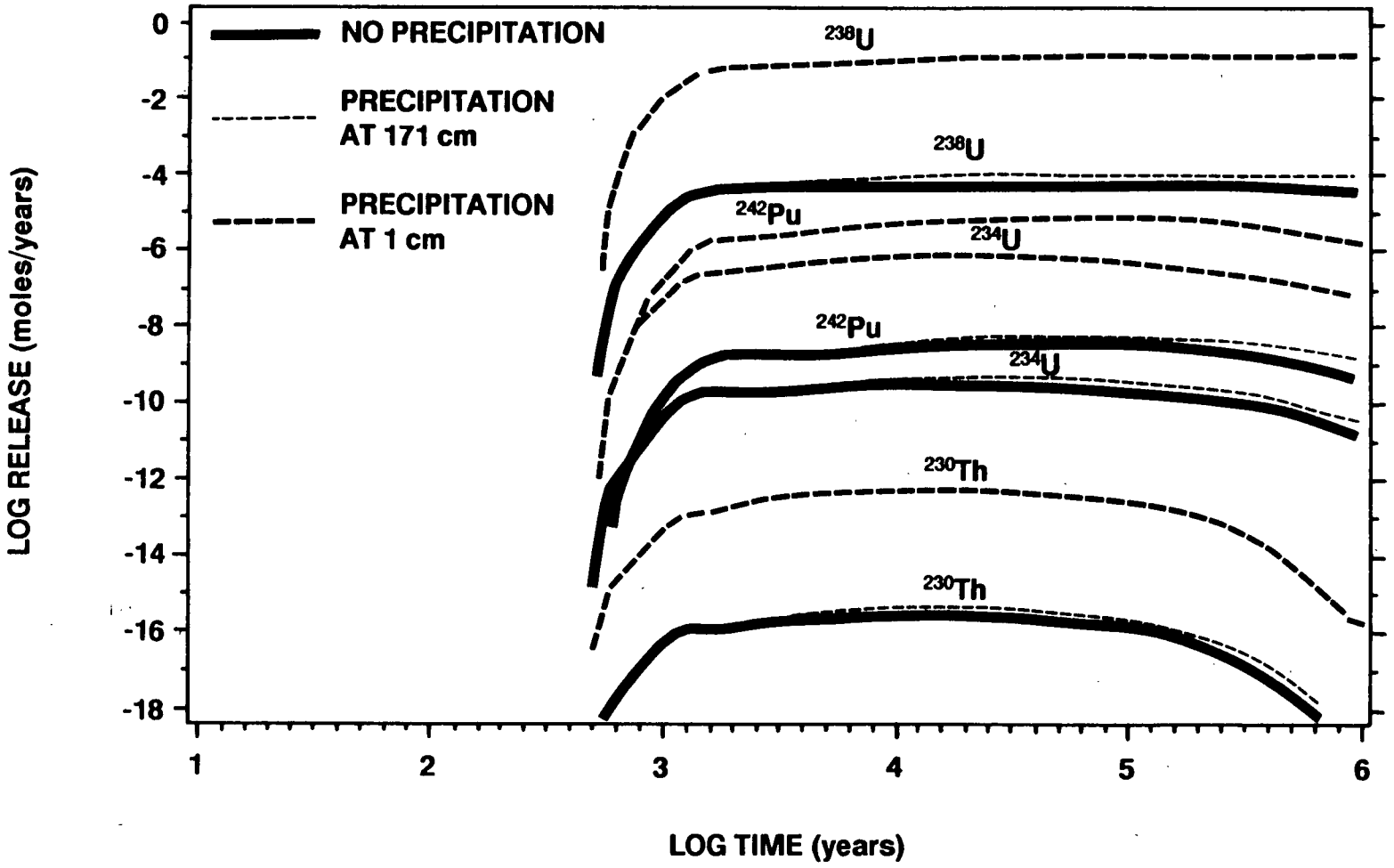
EFFECT OF STABILITY OF UO_2 MATRIX ON RELEASE (POINT FAILURE AT 300 YEARS)



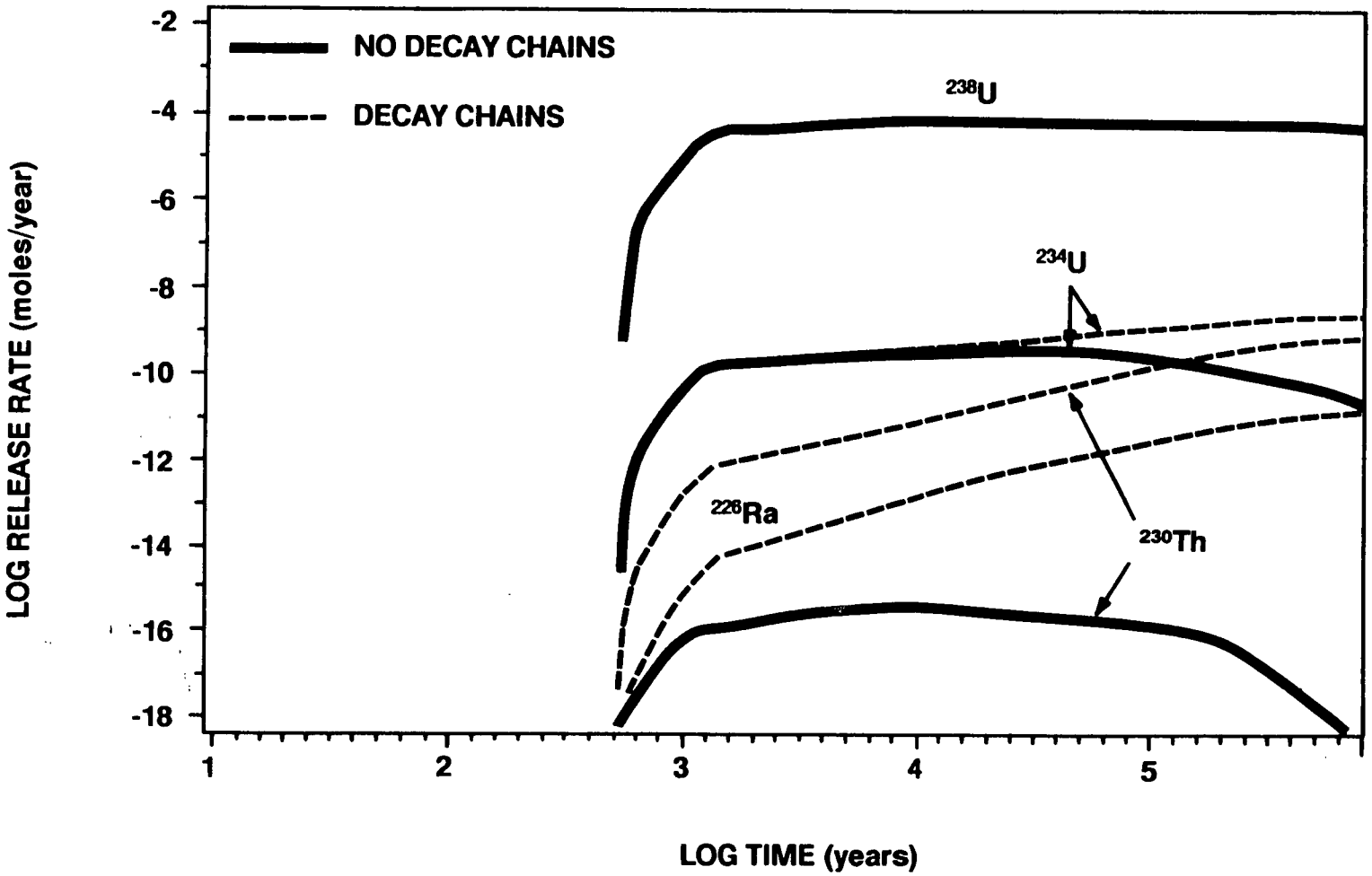
EFFECT OF DISTRIBUTED CONTAINMENT FAILURES ON EBS RELEASE



EFFECT OF PRECIPITATION



EFFECT OF DECAY-CHAIN IN-GROWTH



SCOPE OF PRESENTATION

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BENCHMARK OF AREST AND SYVAC-VAULT CODES

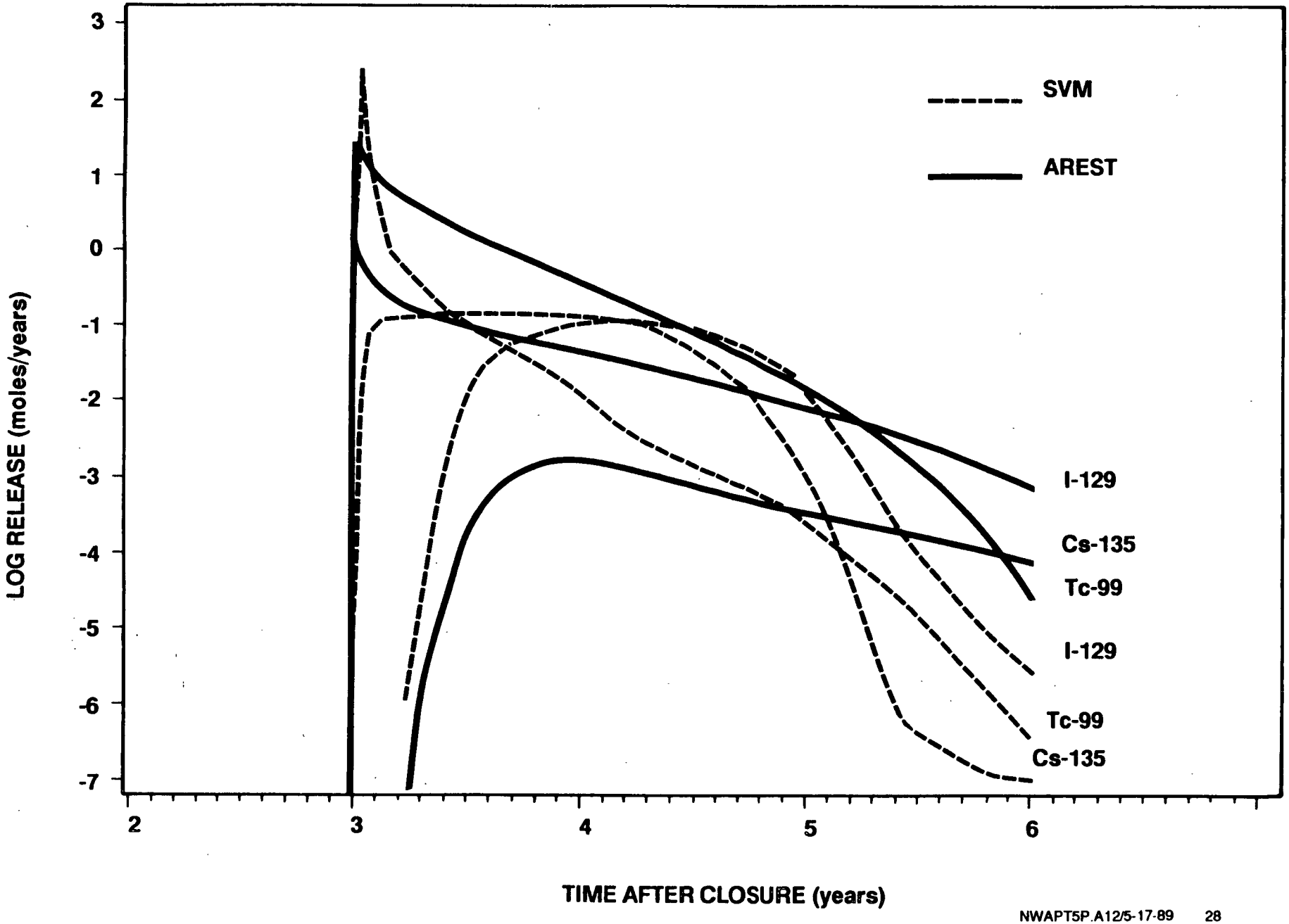
Subnodal

- ESTABLISH CREDIBILITY OF CODES FOR PREDICTIVE PERFORMANCE ASSESSMENT OF WASTE PACKAGES
- IDENTIFY DEFICIENCIES
- IDENTIFY FUTURE IMPROVEMENTS
- FORM A BETTER UNDERSTANDING OF BOTH APPROACHES

COMPARISON OF RELEASE MODELS AND ASSUMPTIONS

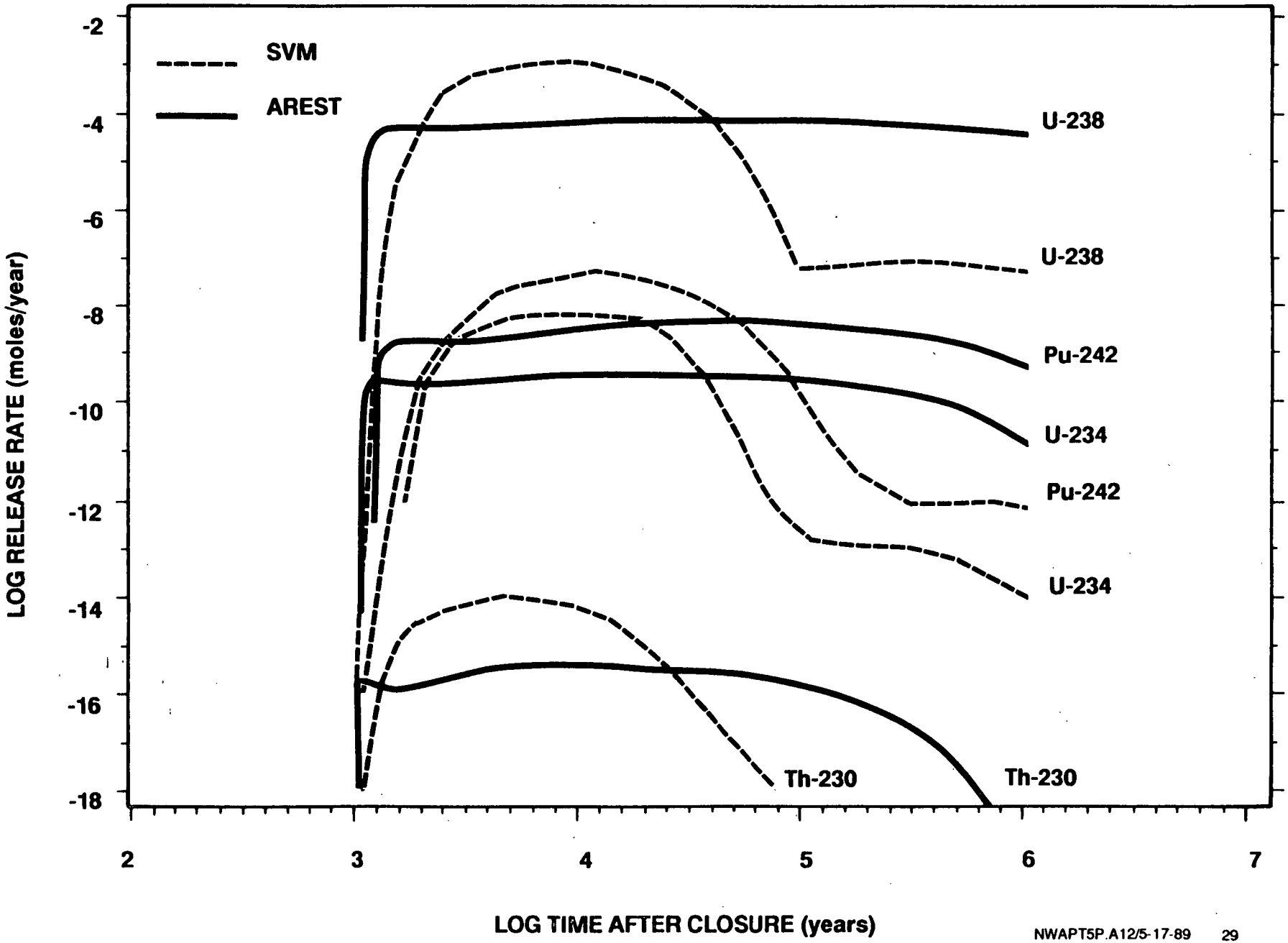
AREST	SYVAC-VAULT (SVM)
• SPHERICAL WP GEOMETRY	PLANAR WP GEOMETRY
• EXACT ANALYTICAL SOLUTION OF DIFFUSIONAL MASS-TRANSFER	APPROXIMATE TRANSIENT SOLUTION (EXACT FOR STEADY-STATE)
• EBS MODELED AS SUMMATION OF INDIVIDUAL WASTE PACKAGES	EBS MODELED AS A SINGLE, CONTINUOUS "SLAB" SOURCE
• SEMI-INFINITE HOST-ROCK THICKNESS	FINITE (500 METERS) HOST-ROCK THICKNESS
• INITIAL CONCENTRATION OF NUCLIDES IN HOST ROCK EQUALS ZERO	SAME
• SOLUBILITY LIMITS ATTAINED AT TIME OF CONTAINMENT FAILURE	SAME
• NO DECAY-CHAIN GROW-IN	SAME
• NO PRECIPITATION	SAME

COMPARISON OF GAP RELEASE

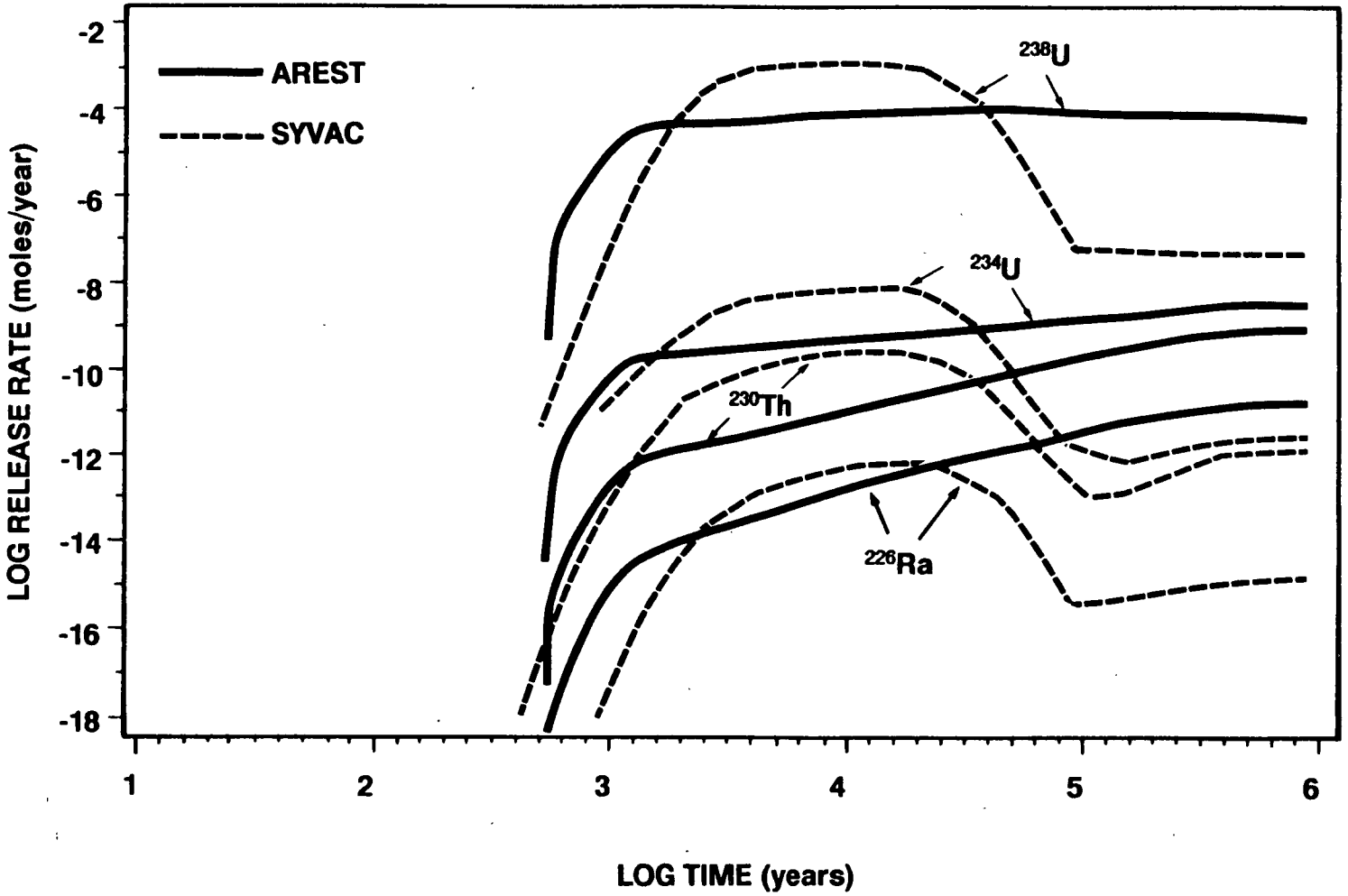


Wet continuous case does not apply to Yucca

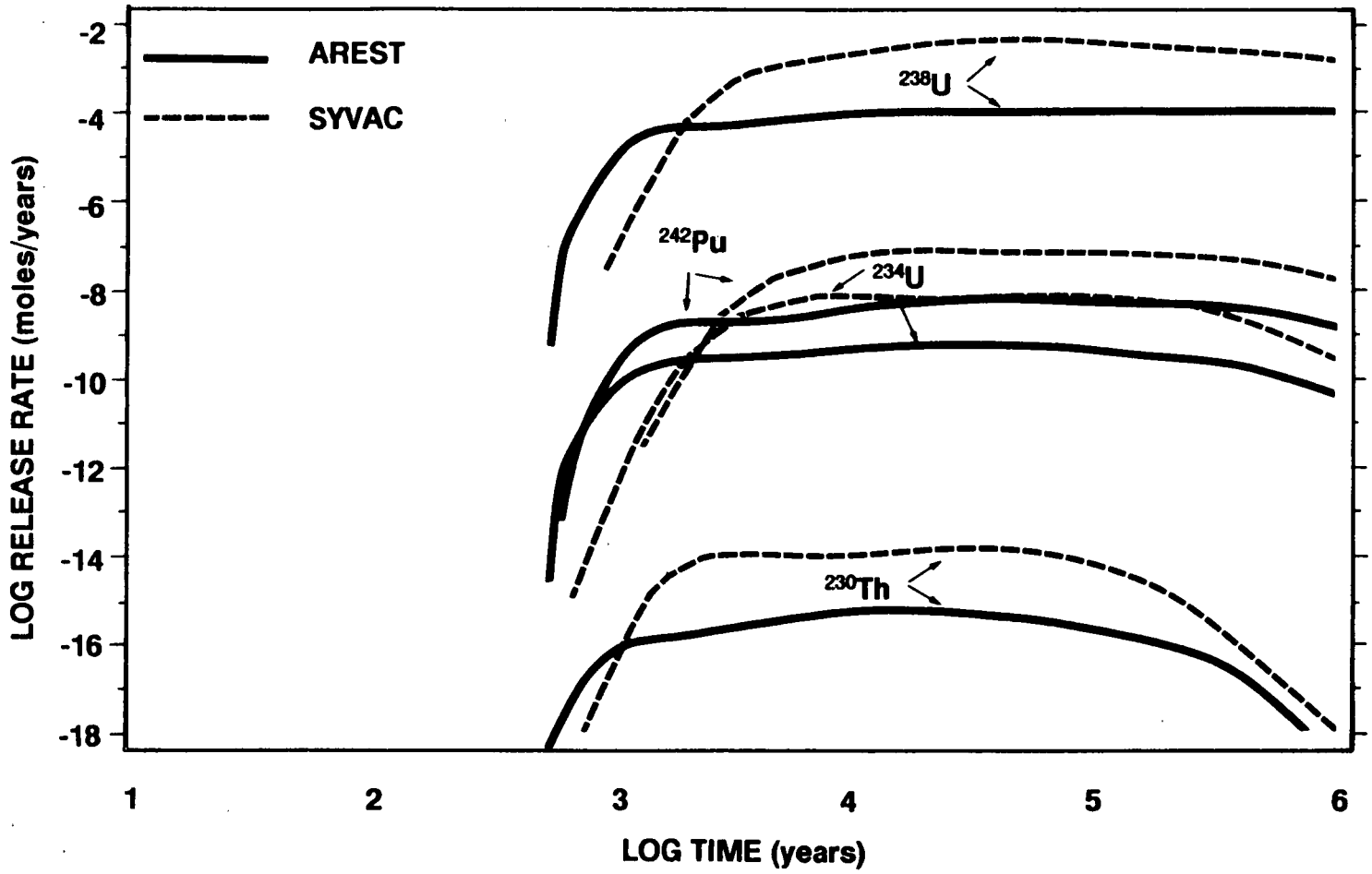
COMPARISON OF MATRIX RELEASE: BASE CASE



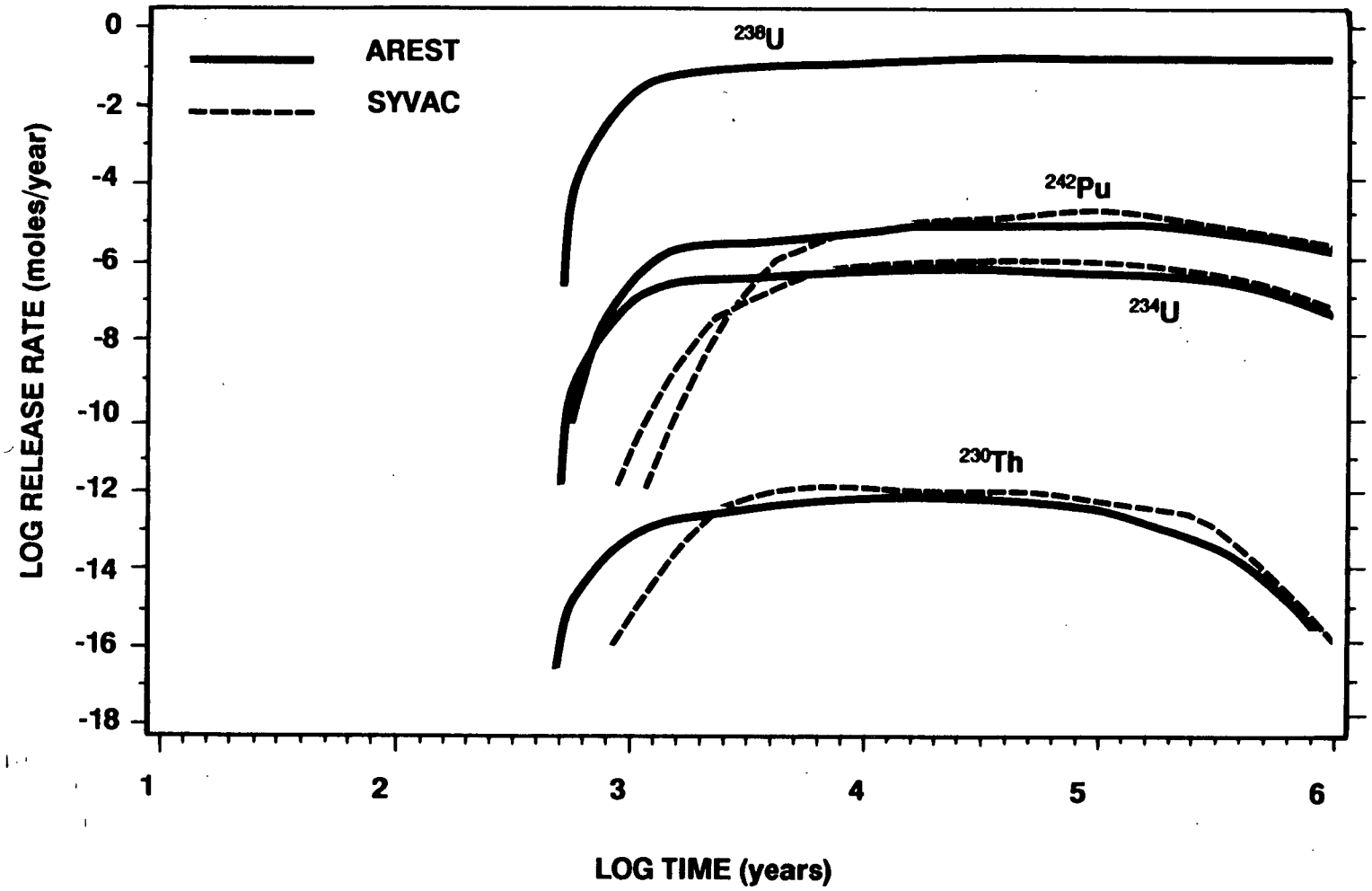
COMPARISON OF MATRIX RELEASE: DECAY-CHAIN IN-GROWTH



COMPARISON OF MATRIX RELEASE: PRECIPITATION AT HOST ROCK



COMPARISON OF MATRIX RELEASE: PRECIPITATION NEAR WASTE FORM



CONCLUSIONS FROM BENCHMARK TESTS

- RESULTS IN REASONABLE AGREEMENT
- DIFFERENCES WERE ANTICIPATED AND ARE ATTRIBUTABLE TO:
  - ANALYTICAL FORMATION
    - * EXACT VS. APPROXIMATE TRANSIENT SOLUTION
  - GEOMETRY
    - * PLANAR VS. SPHERICAL
  - BOUNDARY CONDITIONS
    - * SEMI-INFINITE VS. FINITE ROCK THICKNESS
    - * USE OF CONCENTRATION-DEPENDENT (TIME-DEPENDENT) MASS-TRANSFER COEFFICIENTS

SCOPE OF PRESENTATION

- STRUCTURE OF AREST CODE
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FUTURE ACTIVITIES

- MODIFICATIONS TO CONTAINMENT MODELS
  - ALTERNATE CONTAINER MATERIALS
  - CLADDING FAILURE
- ENHANCEMENTS TO RELEASE MODELS
- FURTHER EVALUATION OF COUPLED PROCESSES
  - THERMAL-HYDROLOGICAL
  - THERMAL-MECHANICAL
  - GEOCHEMICAL-RADIATION
- SCALE EFFECTS ON NEAR-FIELD ANALYSIS
- BENCHMARK COMPARISON ON TEST PROBLEMS
- SENSITIVITY ANALYSES