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

PRESENTATION TO THE NUCLEAR WASTE TECHNICAL REVIEW BOARD

SUBJECT: MODELS OF WASTE PACKAGE BEHAVIOR IN A REPOSITORY ENVIRONMENT

PRESENTER: DR. THOMAS H. PIGFORD

PRESENTER'S TITLE AND ORGANIZATION: DEPARTMENT OF NUCLEAR ENGINEERING & LAWRENCE BERKELEY LAB, UNIVERSITY OF CALIFORNIA, BERKELEY, CA.

PRESENTER'S TELEPHONE NUMBER: (415) 642-6469

MAY 16-17, 1989

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SCOPE OF PRESENTATION

- OBJECTIVES
- DEVELOPMENT OF MODELS
- RESULTS OF CURRENT WORK
- FUTURE ACTIVITIES

THE DESIGN OBJECTIVE

TO DESIGN A REPOSITORY THAT PERFORMS SUFFICIENTLY WELL WHEN MEASURED AGAINST CRITERIA FOR SATISFACTORY LONG-TERM PROTECTION OF PUBLIC HEALTH AND SAFETY

THE PURPOSE OF PERFORMANCE PREDICTIONS

- TO MAKE RELIABLE PREDICTIONS THAT PERFORMANCE WILL NOT FALL OUTSIDE THE CRITERIA FOR ACCEPTABILITY
- PREDICTING ALL DETAILS OF REPOSITORY PERFORMANCE IS NEITHER NECESSARY OR ACHIEVABLE

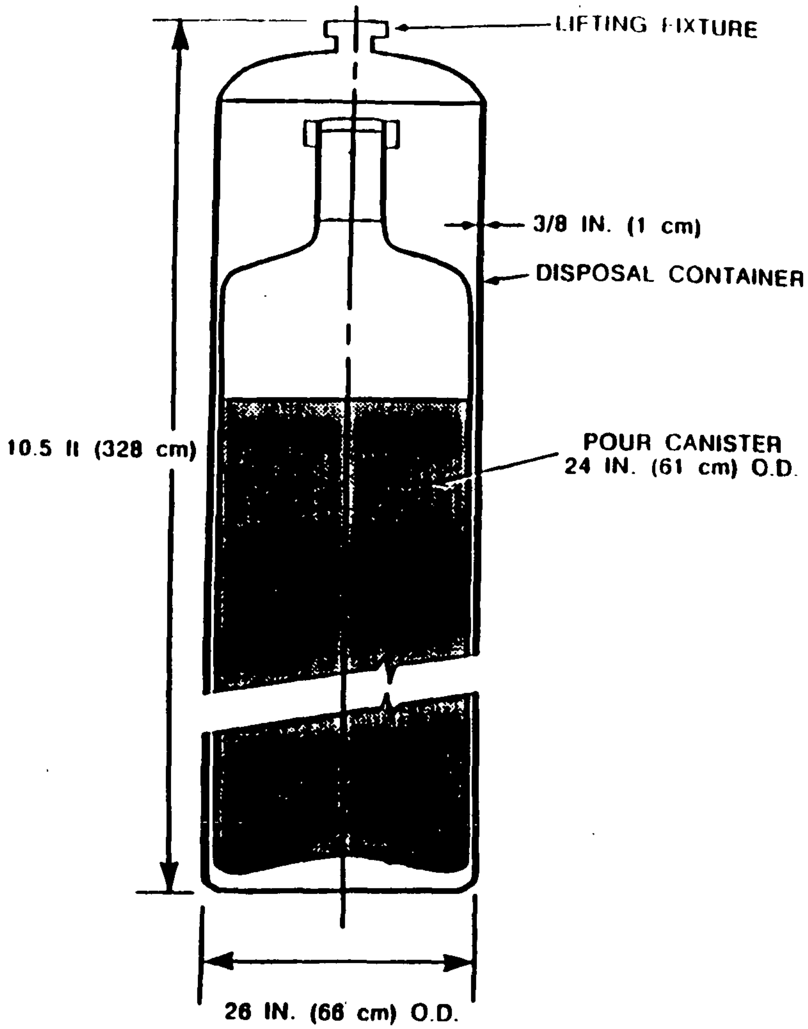
PREDICTIVE RELIABILTY

PREDICTIVE RELIABILTY IN DESIGN DEPENDS ON:

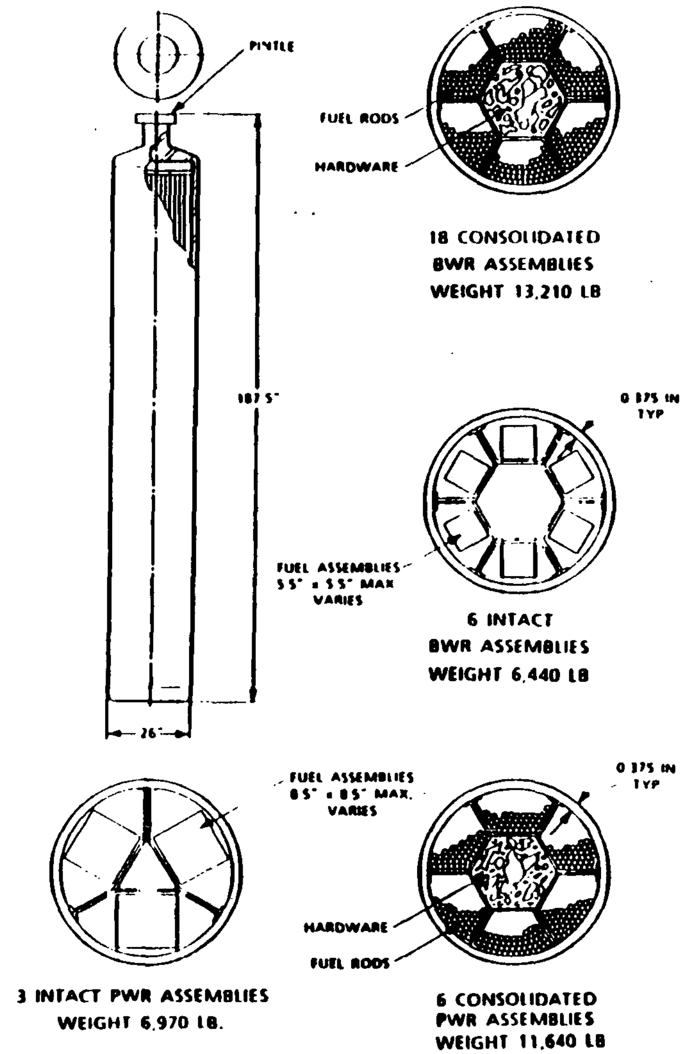
- CLEAR AND RELIABLE CRITERIA FOR ACCEPTABLE PERFORMANCE
- A THEORY THAT CAN RELIABLY PREDICT THE PERFORMANCE DOES NOT FALL OUTSIDE THE CRITERIA FOR ACCEPTABLE PERFORMANCE
- RELIABLE PARAMETER VALUES TO APPLY THE THEORY

CONCEPTUAL WASTE PACKAGE DESIGNS FOR HIGH-LEVEL WASTE AND SPENT NUCLEAR FUEL

HIGH-LEVEL WASTE CONTAINER



SPENT NUCLEAR FUEL CONTAINER



THREE GENERAL MODELS FOR WASTE PACKAGE RELEASES

1. DRY { most likely case
2. WET-DRIP
3. WET-CONTINUOUS

1. DRY CASE FOR WASTE PACKAGE RELEASES

A. SOME CONTAINERS FAIL, ALLOWING RADIOACTIVE GASES TO ESCAPE
(e.g., ^{3}H, ^{14}C, ^{85}Kr, ^{129}I)

B. NO WATER ENTERS THE PENETRATIONS IN THE FAILED CONTAINERS. NO NON-VOLATILE RADIONUCLIDES ARE RELEASED

2. WET-DRIP CASE

- BOUNDING CALCULATIONS OF RADIONUCLIDE RELEASE RATES TO GROUND WATER FOR INDIVIDUAL WASTE PACKAGES AT YUCCA MOUNTAIN
- ASSUME NO CLADDING BARRIER
- ASSUME GROUND WATER ENTERS AND LEAVES DEFECTIVE WASTE PACKAGE
- BATHTUB AND FLOW-THROUGH MODELS (ASSUMING NO DIFFUSIVE PATHWAY TO SURROUNDING ROCK)

(a) BULK-FLOW SOLUBILITY-LIMITED (e.g., U, Pu, Np, Am)

$$\dot{m}_i = Q \frac{n_i}{n_e} N_e^*, \quad f_i = \frac{\dot{m}_i}{M_i}$$

<u>WHERE</u>

f_i IS THE FRACTIONAL RELEASE RATE OF SPECIES i
n_e IS THE CONCENTRATION OF ELEMENT CONTAINING SPECIES i IN WASTE
n_i IS THE CONCENTRATION OF ISOTOPE i IN WASTE
$\dot{m}_i$ IS THE RELEASE RATE OF SPECIES i
M_i IS THE 1,000-YEAR INVENTORY OF SPECIES i
N^*_e IS THE SOLUBILITY OF ELEMENT CONTAINING ISOTOPE i
Q IS THE VOLUMETRIC FLOW RATE OF GROUND WATER PER WASTE PACKAGE

2. WET-DRIP CASE

(CONTINUED)

(b) LIMITED BY WASTE-WATER REACTION RATE (e.g., SOLUBLE Tc-99)

$$\dot{m}_i = j_m A \frac{n_i}{n_e}, \quad f_i = \frac{\dot{m}_i}{M_i}$$

WHERE j_m IS THE RATE OF SOLID-SOLID ALTERATION OF THE WASTE MATRIX, (e.g., UO_2 (s) → U_3O_7 (s)), PER UNIT AREA
A IS THE SURFACE AREA OF WASTE EXPOSED TO GROUND WATER

2. WET-DRIP CASE

(CONTINUED)

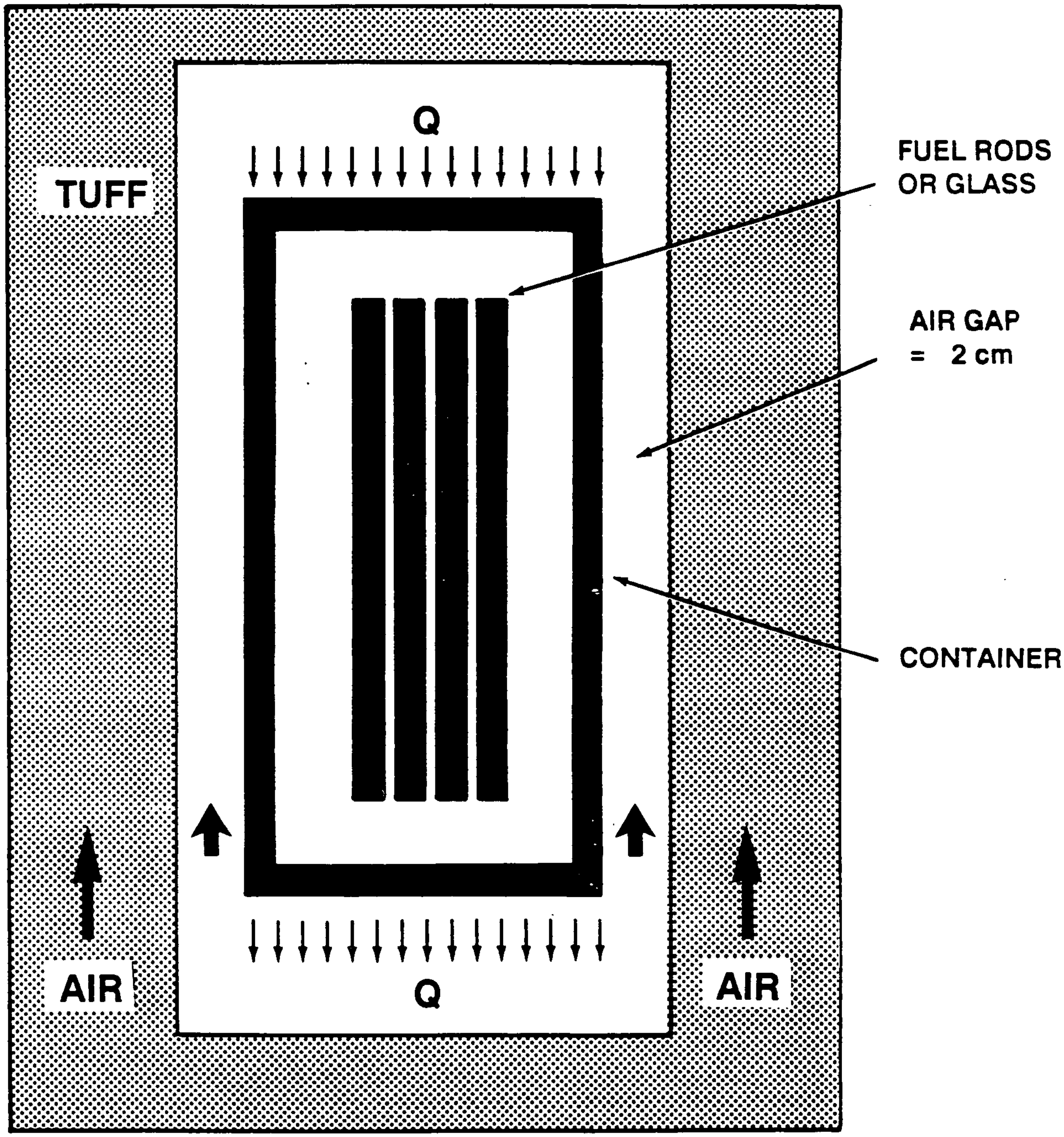
(c) READILY SOLUBLE SPECIES (e.g., Cs, I, not in UO_2 MATRIX)

$$\dot{m}_{is} = M_{is}\frac{d\psi}{dt}, \quad f_{is} = \frac{\dot{m}_{is}}{M_i}$$

WHERE

$\frac{d\psi}{dt}$ IS THE FRACTION OF SOLUBLE INVENTORY M_{is} EXPOSED TO WATER PER UNIT TIME

KEY PARAMETERS: M_{is}, M_i, $\frac{d\psi}{dt}$



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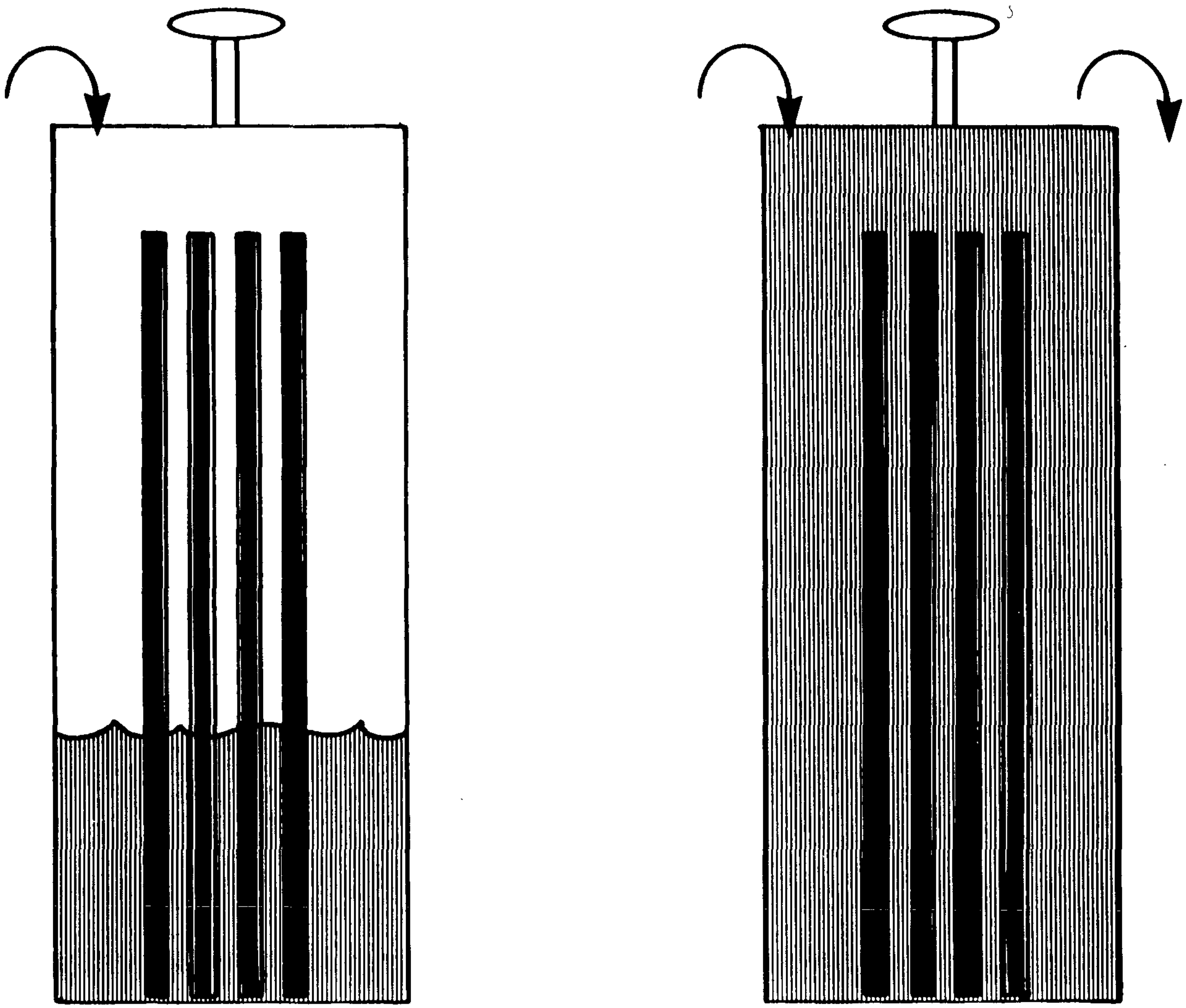
WASTE PACKAGE IN UNSATURATED TUFF
WET-DRIP CASE
(POST-THERMAL PERIOD)
$Q \geq 0$

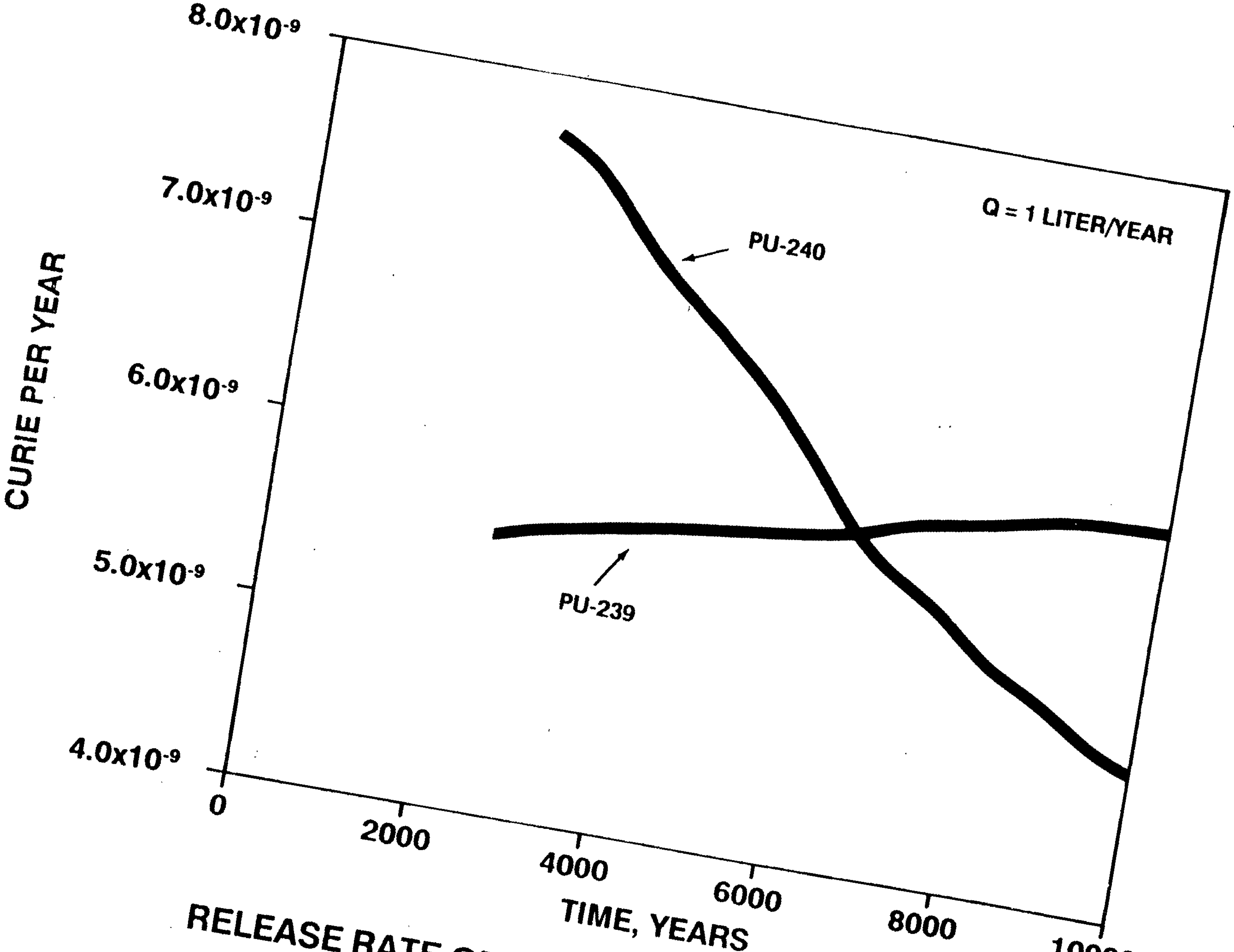
Livermore sponsored

WET-DRIP CASE

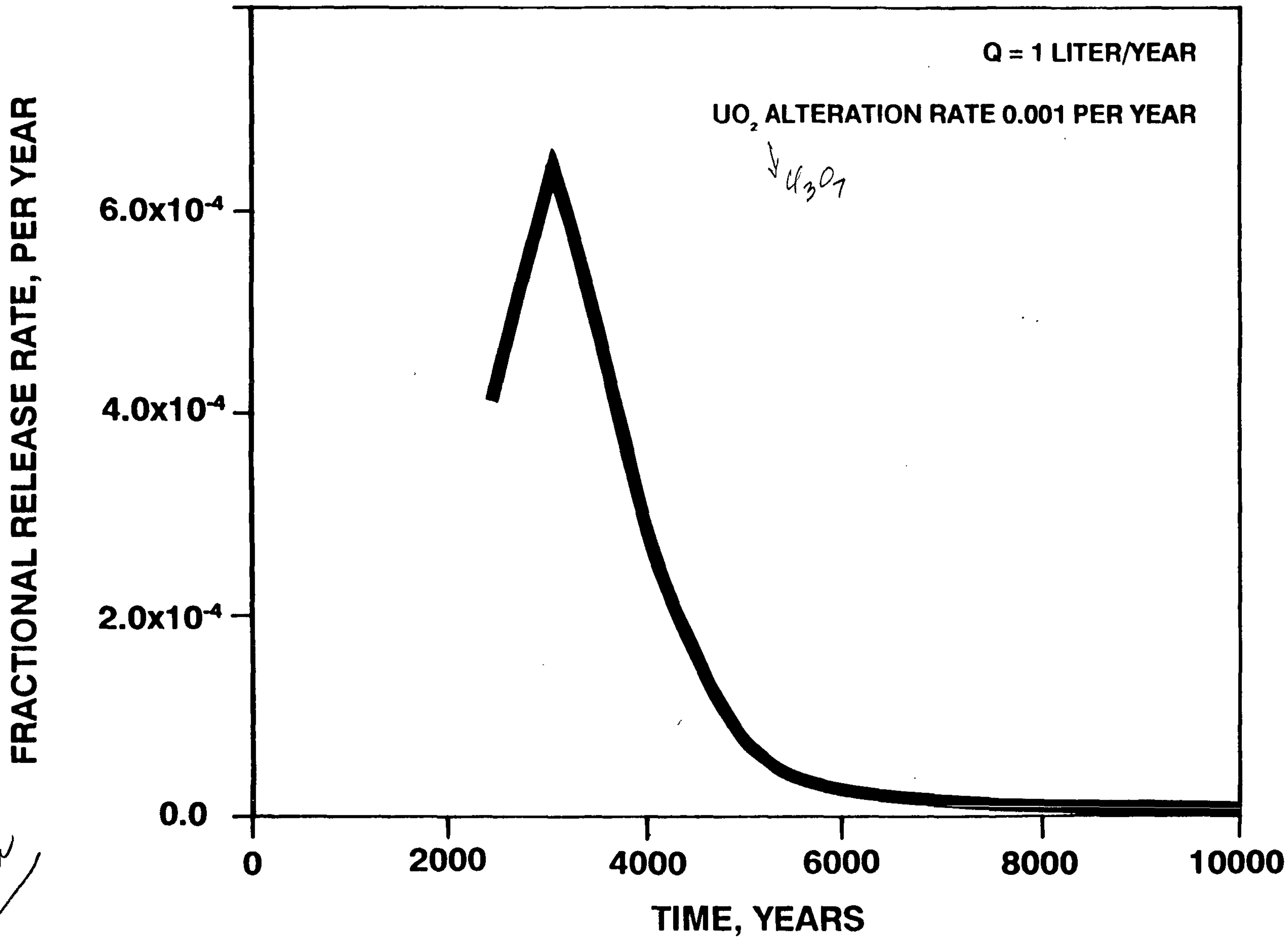
THE "BATHTUB" SCENARIO INVOLVES BREACHES THAT ALLOW WATER TO ENTER AND FILL THE PACKAGE, IMMERSING THE WASTE FORM



FILLING PACKAGE **FILLED PACKAGE**



RELEASE RATE OF Pu-239 & Pu-240, BATHTUB MODEL
SOURCE: O'CONNELL, 1989



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FRACTIONAL RELEASE RATE OF Tc-99 BATHTUB MODEL
SOURCE: O'CONNELL, 1989

3. WET-CONTINUOUS CASE

- DIFFUSIVE-ADVECTIVE MASS TRANSFER - DETAILED ANALYTIC SOLUTIONS
- PRESENT ANALYSES ASSUME WASTE CONTAINER AND FUEL CLADDING ARE NOT PRESENT
- ASSUMES A CONTINUOUS LIQUID DIFFUSION PATHWAY FROM THE WASTE TO THE TUFF

  (a) SATURATION CONCENTRATION OF SPECIES i AT WASTE SURFACE

  COMPLETE TIME-DEPENDENT ANALYTIC SOLUTIONS FOR SINGLE SPECIES OR DECAY CHAINS, FOR WASTE IN CONTACT WITH TUFF, OR SURROUNDED BY BACKFILL AND TUFF, NO ARBITRARY OR ADJUSTABLE PARAMETERS

(a) SATURATION CONCENTRATION OF SPECIES i AT WASTE SURFACE

(CONTINUED)

KEY PARAMETERS FOR THE LOW-FLOW AT YUCCA MOUNTAIN, ASSUMING GROUND WATER IN POROUS MEDIA ONLY

- D COEFFICIENT OF MOLECULAR DIFFUSION IN PORE WATER
- N^*_e ELEMENTAL SOLUBILITY FOR THE SPECIES
- R RADIUS OF SPHERICAL-EQUIVALENT WASTE SOLID
- n_e CONCENTRATION OF ELEMENT CONTAINING SPECIES i IN WASTE
- n_i CONCENTRATION OF ISOTOPE i IN WASTE
- $\dot{m}_i$ RELEASE RATE OF SPECIES i
- M_i 1,000-YEAR INVENTORY OF SPECIES i
- ϵ POROSITY
- λ DECAY CONSTANT
- K RETARDATION FACTOR DUE TO SORPTION
- ℓ THICKNESS OF BACKFILL, IF PRESENT
- S MOISTURE CONTENT

EXTENDED SOLUTIONS INCLUDE EFFECT OF TEMPERATURE CHANGES DUE TO REPOSITORY HEATING AND SUBSEQUENT COOLING.

IF GROUND WATER EXISTS IN THE FRACTURES AND IN POROUS ROCK, ADDITIONAL PARAMETERS ARE:

- FRACTURE SPACING
- FRACTURE APERTURE

GROUND WATER FLOW IS NOT A PARAMETER, UNLESS IT BECOMES MANY ORDERS OF MAGNITUDE GREATER THAN CURRENTLY ESTIMATED FOR YUCCA MOUNTAIN

3. WET-CONTINUOUS CASE

(CONTINUED)

(b) READILY SOLUBLE SPECIES (e.g., Cs, I, NOT IN UO_2 MATRIX)

COMPLETE TIME-DEPENDENT ANALYTIC SOLUTIONS FOR SINGLE SPECIES FOR WASTE IN CONTACT WITH TUFF, OR SURROUNDED BY BACKFILL AND TUFF, NO ARBITRARY OR ADJUSTABLE PARAMETERS

KEY PARAMETERS FOR THE LOW-FLOW AT YUCCA MOUNTAIN

- D COEFFICIENT OF MOLECULAR DIFFUSION IN PORE WATER
- ϵ POROSITY
- V VOLUME WITHIN WASTE PACKAGE THAT CAN BE FILLED WITH WATER
- λ DECAY CONSTANT
- $\bar{K}$ RETARDATION FACTOR DUE TO SORPTION
- ℓ BACKFILL THICKNESS, IF PRESENT
- S MOISTURE CONTENT (FRACTION)
- M_{is} INVENTORY OF SPECIES i IN READILY SOLUBLE FORM

(b) READILY SOLUBLE SPECIES

(CONTINUED)

EXTENDED SOLUTIONS INCLUDE EFFECT OF TEMPERATURE CHANGES DUE TO REPOSITORY HEATING AND SUBSEQUENT COOLING

3. WET-CONTINUOUS CASE

(CONTINUED)

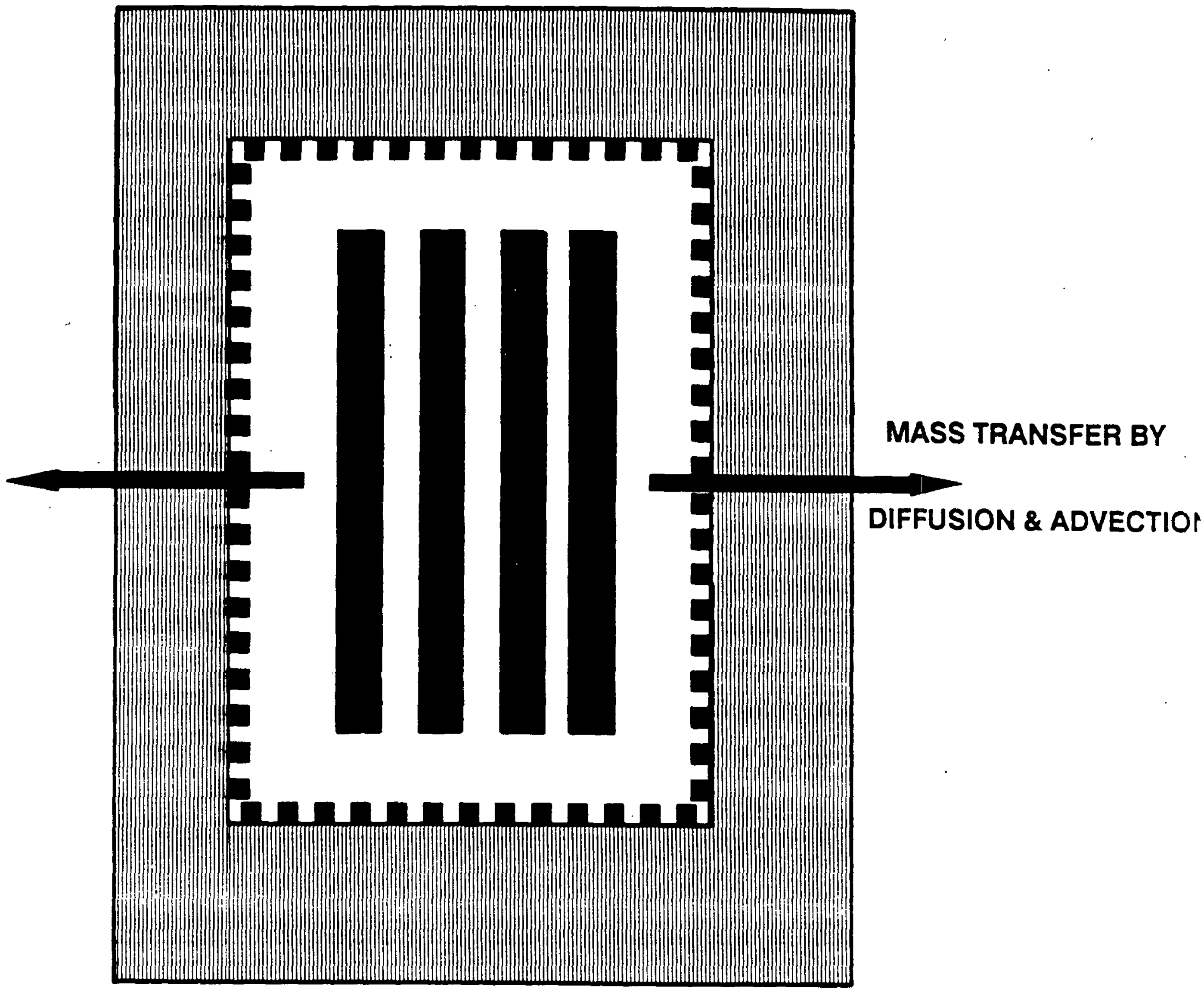
(c) DISSOLUTION OF SPECIES i CONGRUENT WITH THAT OF A DOMINANT LOW-SOLUBILITY SPECIES m

$$f_i = \frac{\dot{m}_i}{M_i} = f_m = \frac{\dot{m}_m}{M_m}, \quad \dot{m}_i = \dot{m}_m \left(\frac{M_i}{M_m}\right)$$

KEY PARAMETERS FOR $\dot{m}_m$ GIVEN IN 3(a)

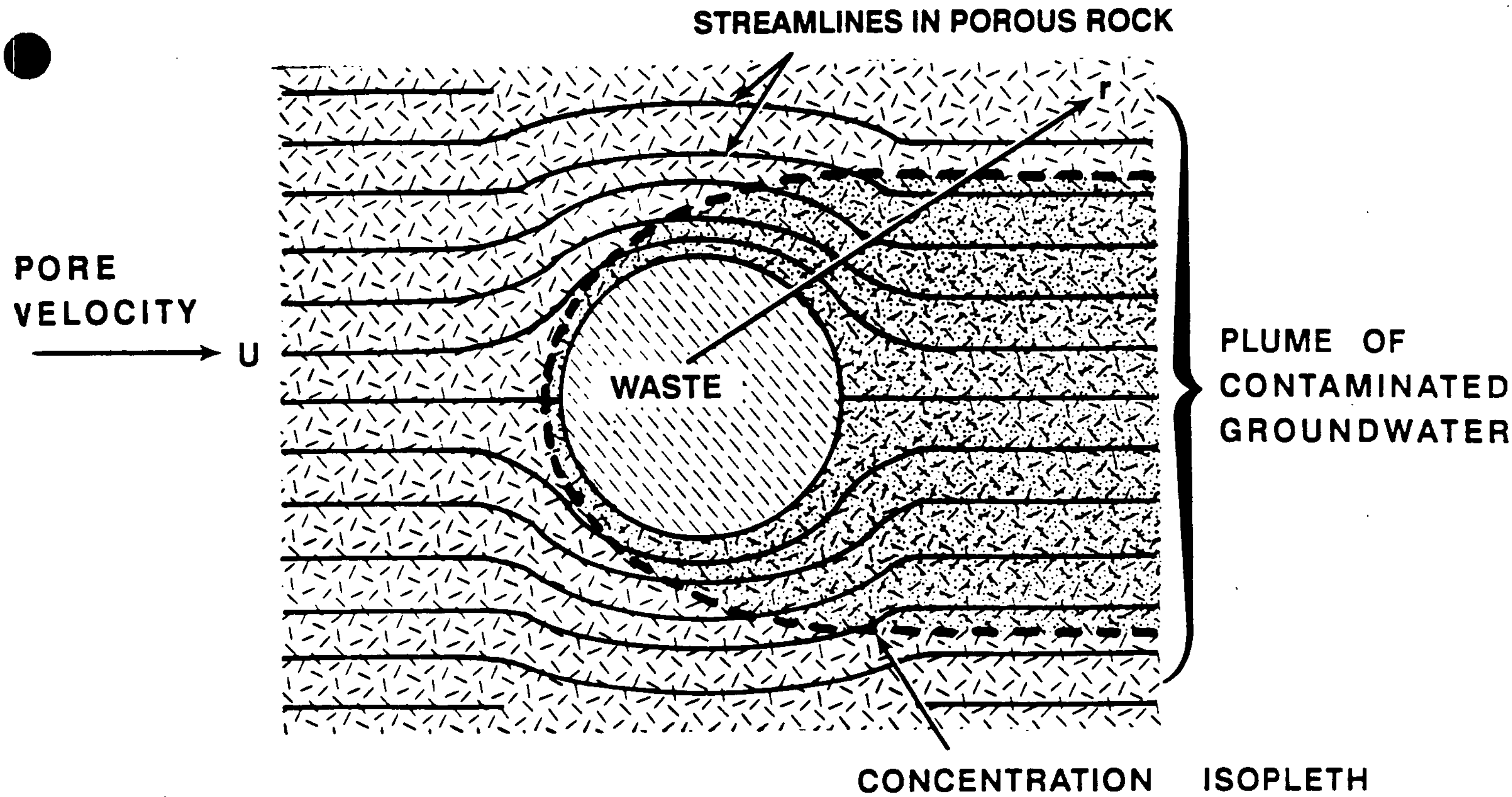
(d) DISSOLUTION OF SPECIES i CONGRUENT WITH THE RATE OF ALTERATION OF THE WASTE MATRIX

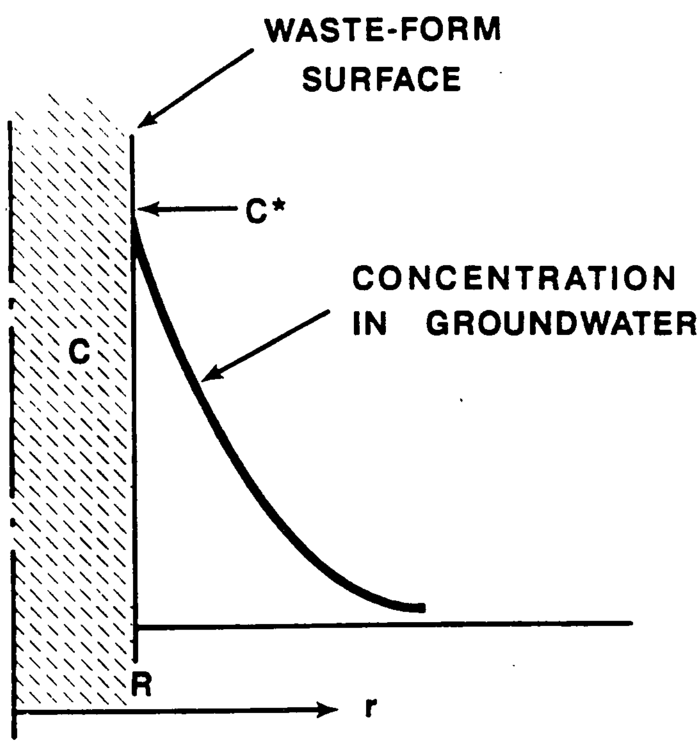
$$\dot{m}_i = j_m \, A \, \frac{n_i}{n_m}, \quad f_i = \frac{\dot{m}_i}{M_i}$$



WET-CONTINUOUS CASE
A WASTE PACKAGE IN SATURATED TUFF

alternative model (Total container failure)





VELOCITY AND CONCENTRATION PROFILES FOR GROUNDWATER FLOWING AROUND A WASTE CYLINDER

3. WET-CONTINUOUS CASE
MASS TRANSFER BY DIFFUSION AND ADVECTION
(NO RADIOACTIVE DECAY)

$$f_j = \frac{8\ N_j^*\ D^{\frac{1}{2}}\ \epsilon\ V^{\frac{1}{2}}\ (1 + R/L)}{(\pi R)^{\frac{3}{2}}\ n_j}, \quad \frac{VR}{D} > 4$$

f_j = FRACTIONAL DISSOLUTION RATE OF SPECIES j

N_j^* = SATURATION CONCENTRATION

D = DIFFUSION COEFFICIENT IN GROUND WATER

ϵ = POROSITY

V = GROUND WATER PORE VELOCITY

R = CYLINDER RADIUS

L = CYLINDER LENGTH

n_j = CONCENTRATION IN WASTE SOLID

NOTATION FOR FIGURES

d DIAMETER

D DIFFUSION COEFFICIENT

f_j FRACTIONAL DISSOLUTION RATE OF SPECIES j

h MASS-TRANSFER COEFFICIENT

j_0 FORWARD REACTION RATE

K RETARDATION COEFFICIENT

r RADIUS

t TIME

V GROUND WATER PORE VELOCITY

α $\frac{\text{BACKFILL PERMEABILITY}}{\text{ROCK PERMEABILITY}}$

β $\frac{\text{ROCK POROSITY}}{\text{BACKFILL POROSITY}}$

ε POROSITY

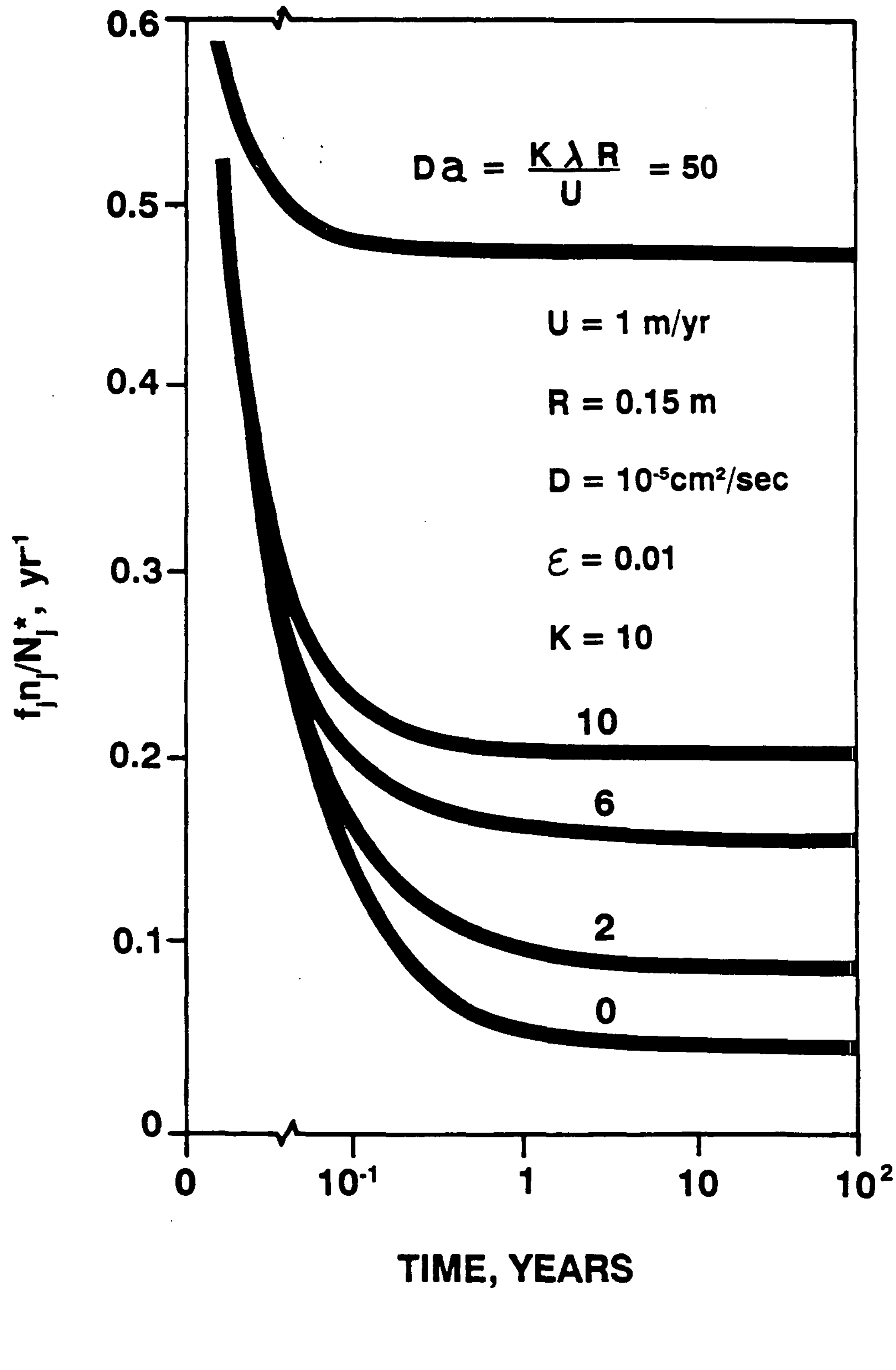
λ RADIOACTIVE DECAY CONSTANT

NOTATION FOR FIGURES

(CONTINUED)

PECLET NUMBER	$Pe = \frac{Vr}{D}$
DAMKÖHLER NUMBER	$Da = \frac{\lambda Kr}{V}$
THIELE MODULUS	$\Lambda = \left(\frac{\lambda d^2 K}{D}\right)^{1/2}$
FOURIER MODULUS	$T = \frac{Dt}{Kd^2}$
SHERWOOD NUMBER	$Sh = \frac{hd}{D\varepsilon}$
REACTION-RATE MODULUS	$R = \frac{j_o r}{\varepsilon D N^*}$

NORMALIZED SOLUBILITY-LIMITED RELEASE RATE AS A FUNCTION OF TIME FLOW ACROSS A WASTE CYLINDER



3. WET-CONTINUOUS CASE MASS TRANSFER BY DIFFUSION (NO RADIOACTIVE DECAY)

$$f_j = \frac{\beta\, \epsilon D N_j^*}{n_j}, \quad \text{as } V \rightarrow 0$$

SPHERE: $\beta = \frac{3}{R^2}$

PROLATE SPHEROID: $\beta = \frac{3e}{b^2 \ln\left(\coth\frac{\alpha_s}{2}\right)}$

e = ECCENTRICITY

b = SEMI-MINOR AXIS

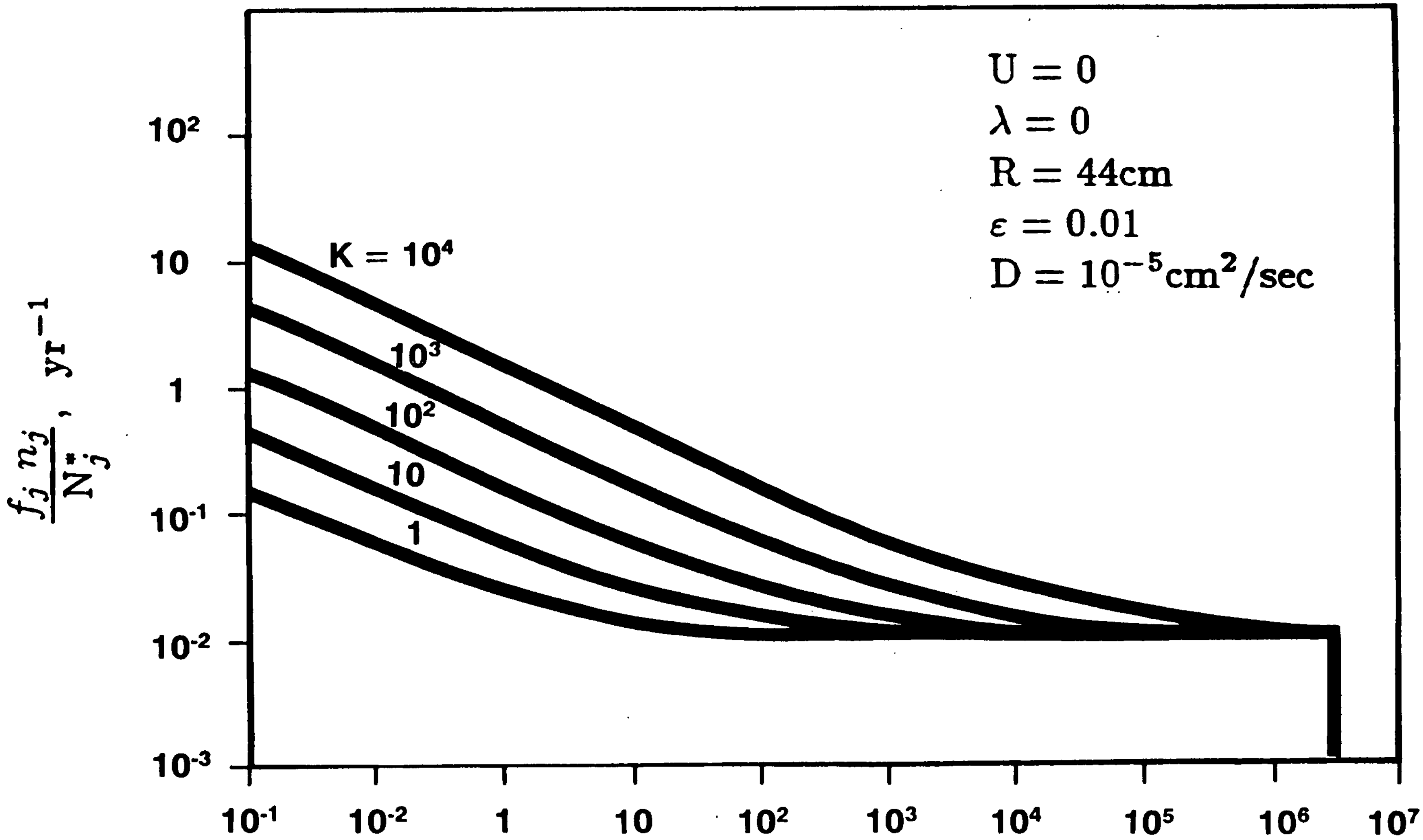
$$\alpha_s = \cosh^{-1}\left(\frac{1}{e}\right)$$

TIME FOR 99% OF STEADY STATE:

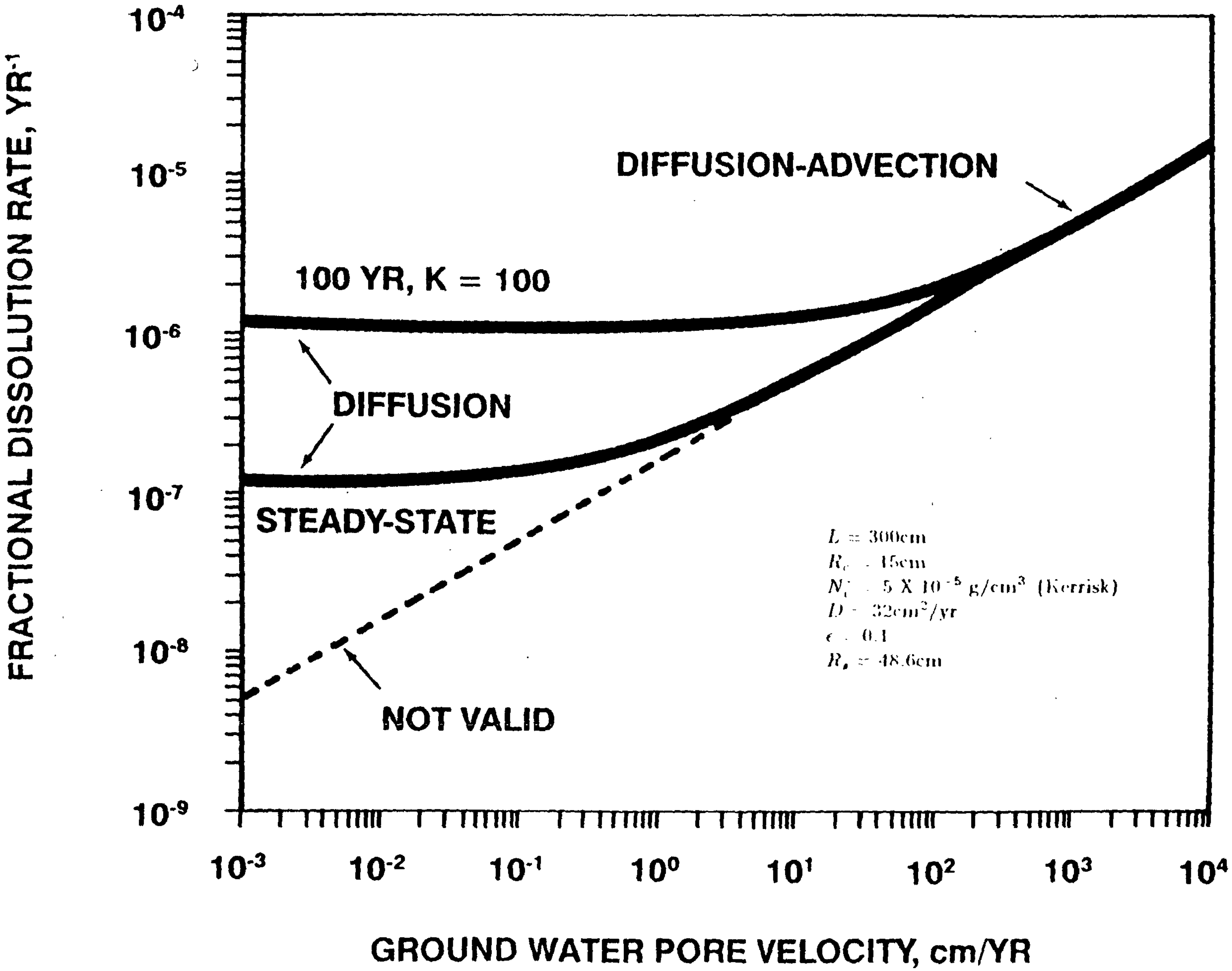
$$t = \frac{10^4\, K b^2}{\pi D}\left[\sinh \alpha_s \ln\left(\coth\frac{\alpha_s}{2}\right)\right]^2$$

K = RETARDATION FACTOR

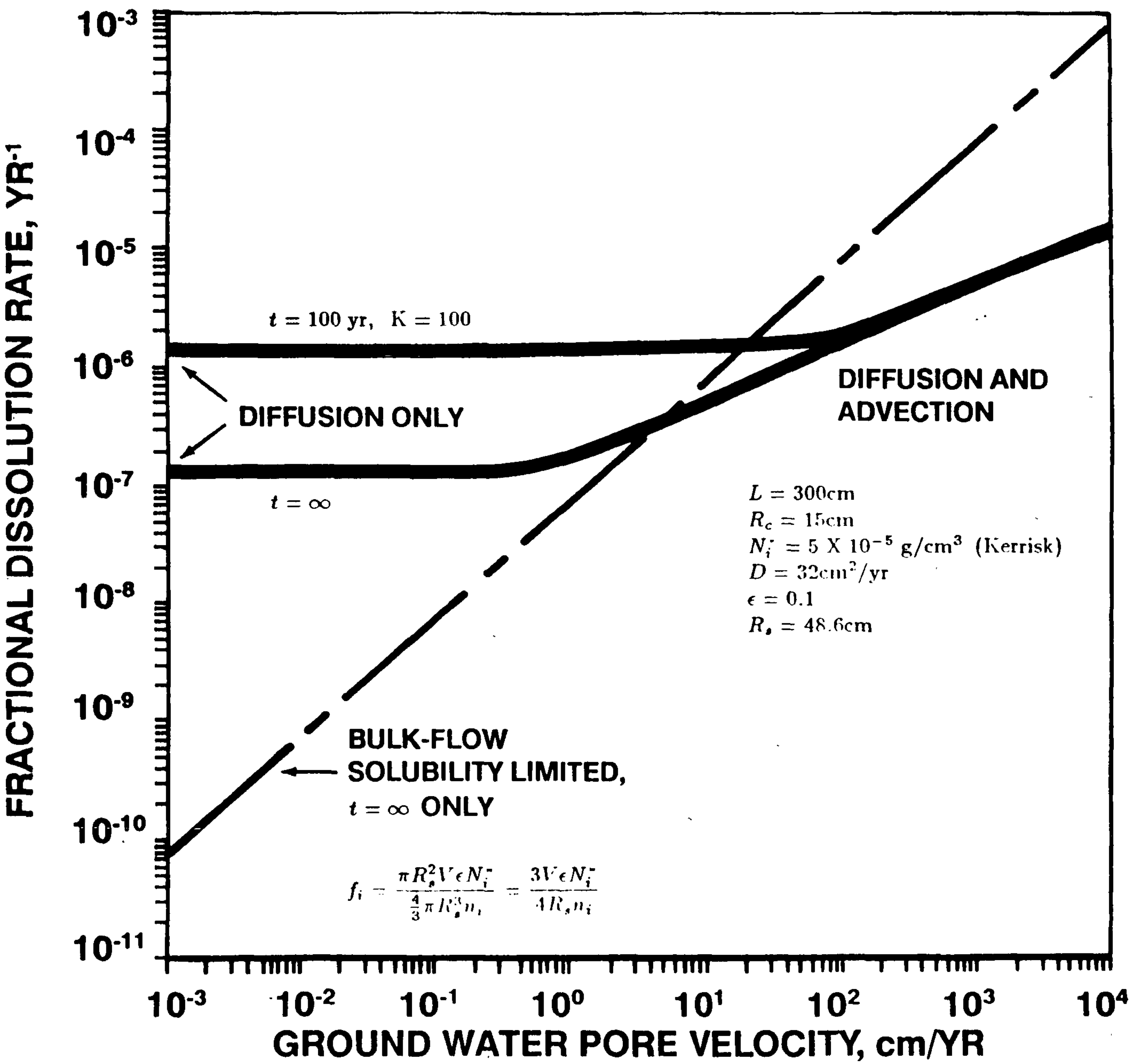
NORMALIZED MASS-TRANSFER RATE AS A FUNCTION OF TIME AND RETARDATION COEFFICIENT (K); DIFFUSION FROM SPHERICAL WASTE FORM



RELEASE RATE AS A FUNCTION OF GROUND WATER VELOCITY
DIFFUSIVE-ADVECTIVE MASS TRANSFER
(UO_2 IN AN OXIDIZING ENVIRONMENT)



COMPARISON OF WET-DRIP AND WET-CONTINUOUS CASES FRACTIONAL RELEASE RATES FOR UO_2 IN AN OXIDIZING ENVIRONMENT



WET-CONTINUOUS CASE, LOW-FLOW RELEASE RATES FOR DEFENSE WASTE BOROSILICATE GLASS

ELEMENT	CONCENTRATION IN WASTE[a] (g/cm^3)	SATURATION CONCENTRATION[b] (g/m^3)	FRACTIONAL RELEASE RATE[c] (PER YEAR)
Si	7.6×10^{-1}	3.2×10^{2}	7.6×10^{-7}
U	5.4×10^{-2}	4.7×10^{-2}	1.6×10^{-9}
Np	5.3×10^{-5}	3.0×10^{-4}	1.0×10^{-8}
Pu	3.0×10^{-4}	3.8×10^{-10}	2.3×10^{-15}
Am	4.1×10^{-7}	1.5×10^{-3}	6.6×10^{-6}
Cs	2.0×10^{-3}	6.2×10^{-1}	5.6×10^{-7}

NOTES:

A. DATA FROM BRUTON, 1987; WASTE DENSITY = 3 g/cm^3

B. DATA FROM BRUTON, 1987, AT 90 C; EXCEPT Cs SOLUBILITY FROM APTED, 1989

C. WASTE CYLINDER 0.3m RADIUS, 2.5m LONG; PORSITY = 0.16; DIFFUSION COEFFICIENT 10^{6} cm^2/s; LOW-FLOW STEADY STATE MASS TRANSFER ANALYSIS

EVOLUTION OF SOLUBILITY DATA FOR SPENT FUEL SOLUBILITY (MOLES/L) AT 25 C

ELEMENT	EA 1986	SCP 1988	LLNL 1989
Am	1×10^{-8}	1×10^{-6}	1.6×10^{-10}
Np	3×10^{-3}	1×10^{-3}	6.3×10^{-6} to 10^{-9}
Pu	1.8×10^{-6}	1×10^{-5}	4×10^{-13} to 1.6×10^{-4} NOTE a. 5×10^{-5} to 2×10^{-6} NOTE b.
U	2.1×10^{-4}	4×10^{-3}	6.3×10^{-5} NOTE c.

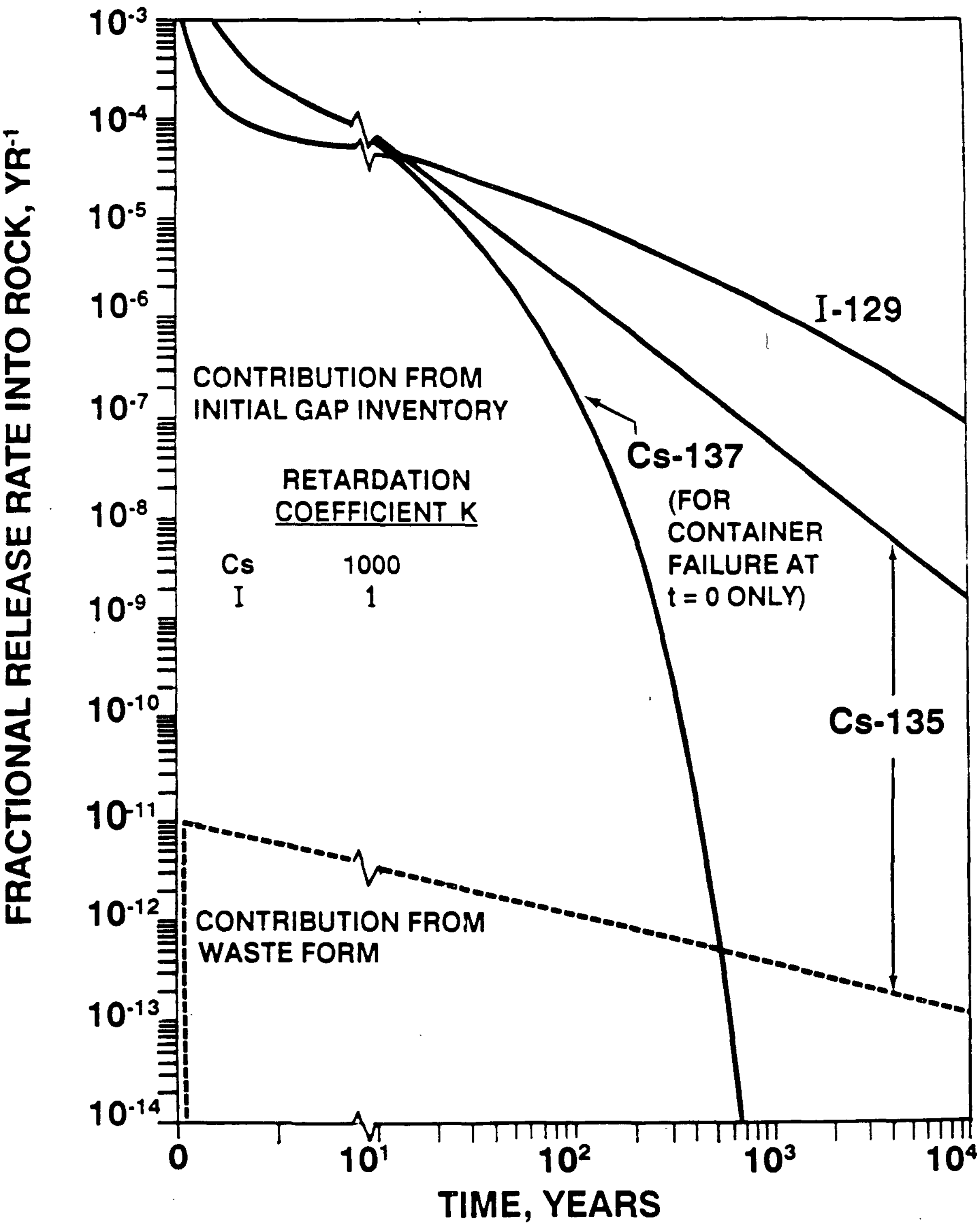
NOTES:

A. AS PuO_2

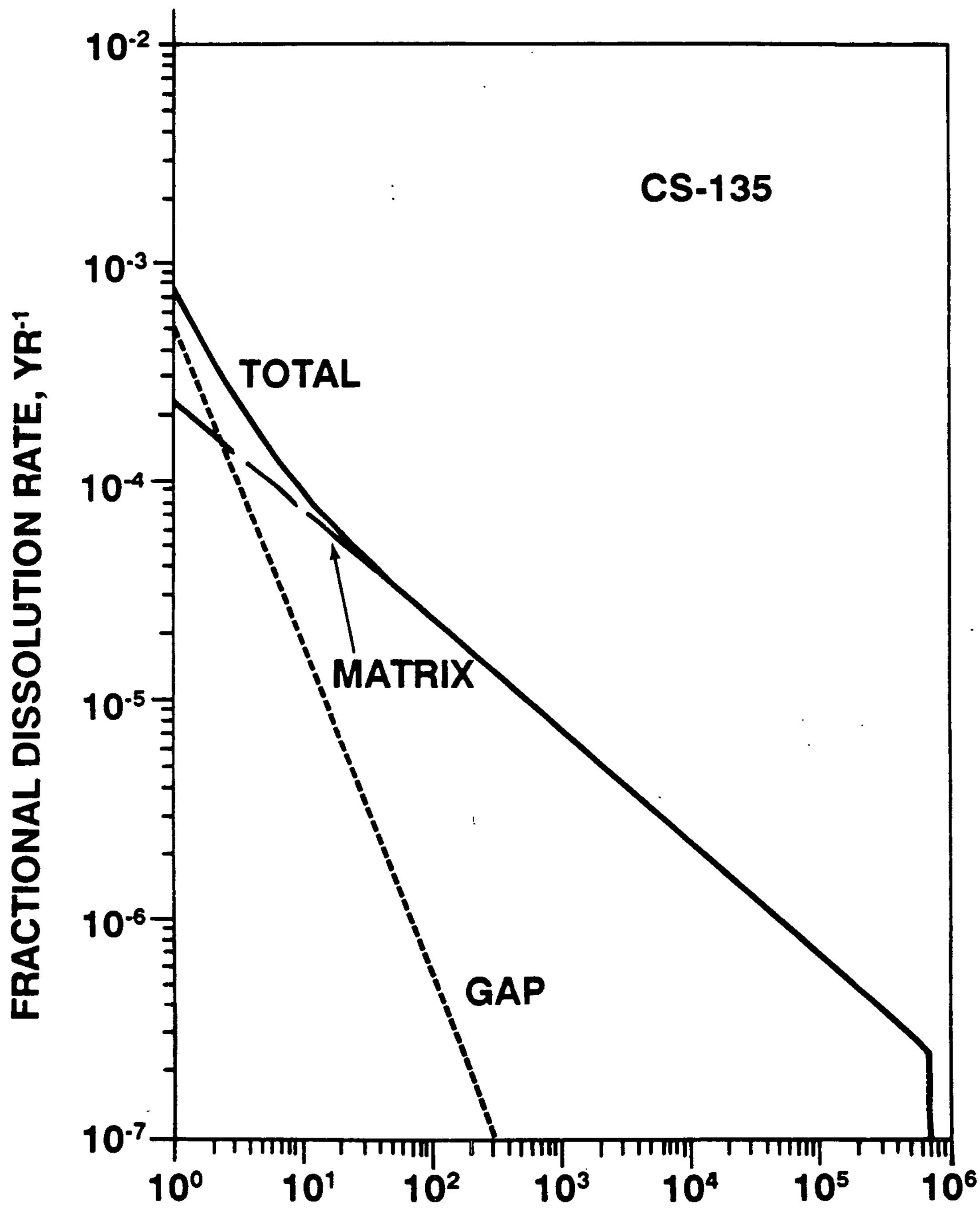
B. AS AMORPHOUS $Pu(OH)_4$

C. IN EQUILIBRIUM WITH ATMOSPHERIC OXYGEN

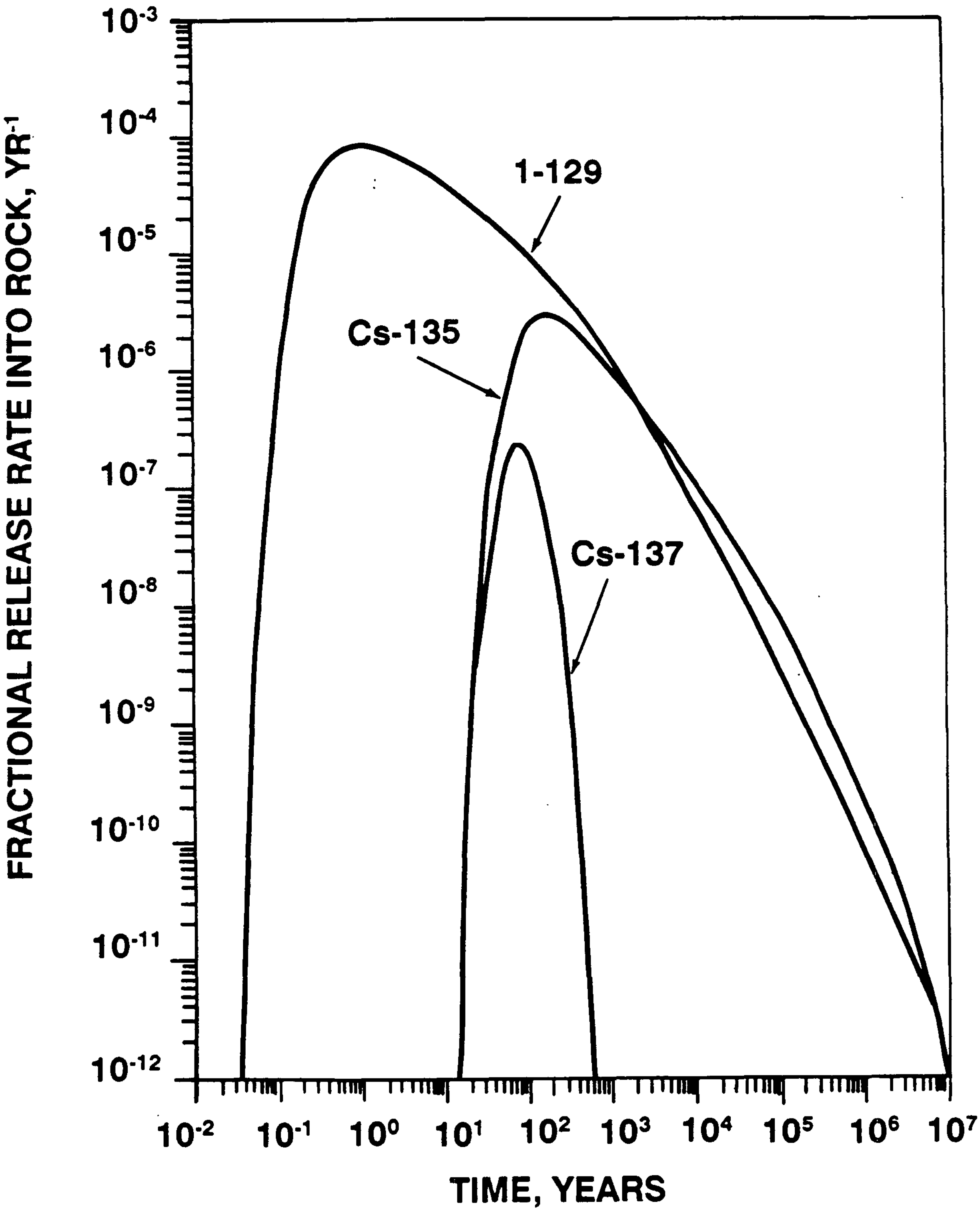
FRACTIONAL RELEASE RATES FROM SPENT FUEL INTO ROCK AS A FUNCTION OF TIME (10cm OF VOID WATER, 1% OF TOTAL CESIUM AND IODINE IS IN GAP, D = 0.12 M^2/YR, NON-OXIDIZING ENVIRONMENT)



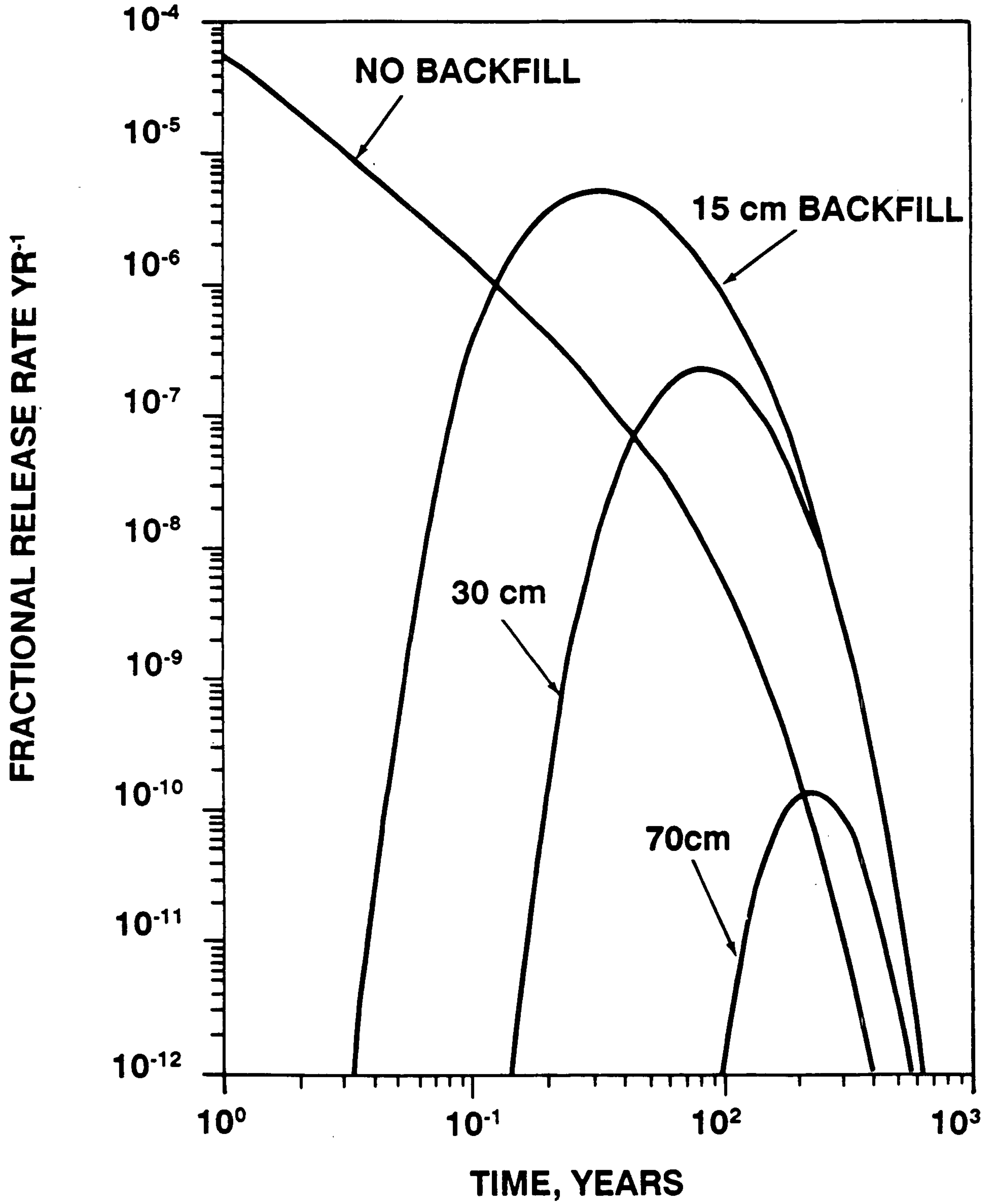
FRACTIONAL RELEASE RATES FROM SPENT FUEL INTO ROCK AS A FUNCTION OF TIME (10cm OF VOID WATER, 1% OF TOTAL CESIUM AND IODINE IS IN GAP, D = 0.12 M^2/YR, OXIDIZING ENVIRONMENT)



RELEASE RATES OF SOLUBLE SPECIES THROUGH 0.3m OF BACKFILL



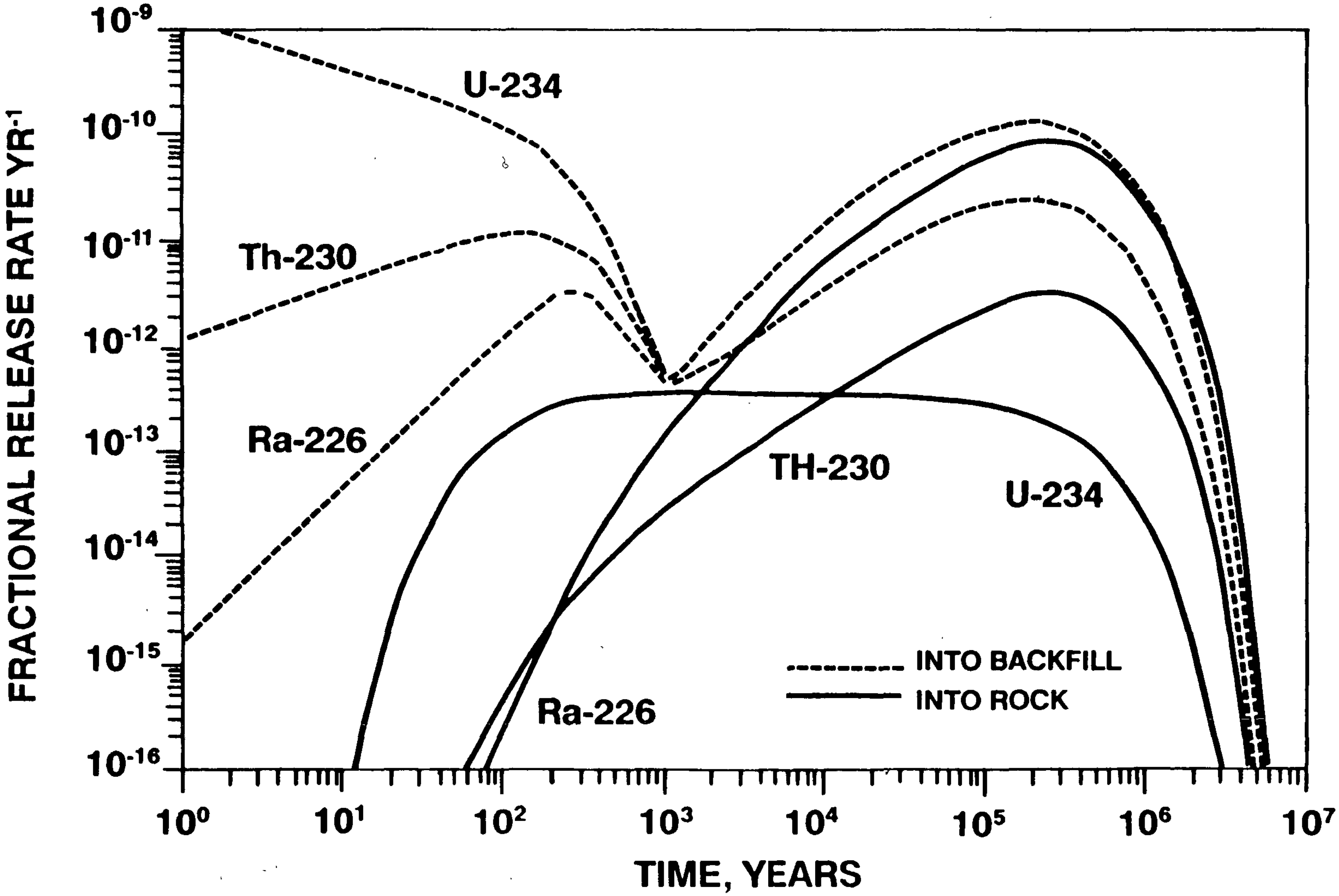
RELEASE RATES OF SOLUBLE Cs-137 SPECIES AS A FUNCTION OF BACKFILL THICKNESS



OTHER USUAL ASSUMPTIONS IN MASS-TRANSFER THEORY

1. EFFECT OF A LIQUID-FILLED ANNULUS BETWEEN WASTE & ROCK
2. EFFECT OF FLOW DIRECTION AND GEOMETRY
3. HYDRODYNAMIC DISPERSION
4. EFFECT OF RADIOACTIVE DECAY
5. LOCAL SORPTION EQUILIBRIUM
6. LINEAR SORPTION: CONSTANT DISTRIBUTION COEFFICIENT, CONSTANT RETARDATION COEFFICIENT
7. SURFACE DIFFUSION
8. INTERFERENCE FROM OTHER WASTE PACKAGES
9. POROUS OR FRACTURED ROCK
10. CONSTANT TEMPERATURE
11. CONSTANT AND UNIFORM CHEMICAL ENVIRONMENT
12. NO RADIOACTIVE DECAY PRECURSOR

FRACTIONAL RELEASE RATES OF A RADIONUCLIDE DECAY CHAIN, NORMALIZED TO 1000 YEAR INVENTORIES



NOTE: Th-230 AND Ra-226 ASSUMED TO BE RELEASED CONGRUENTLY WITH U-234

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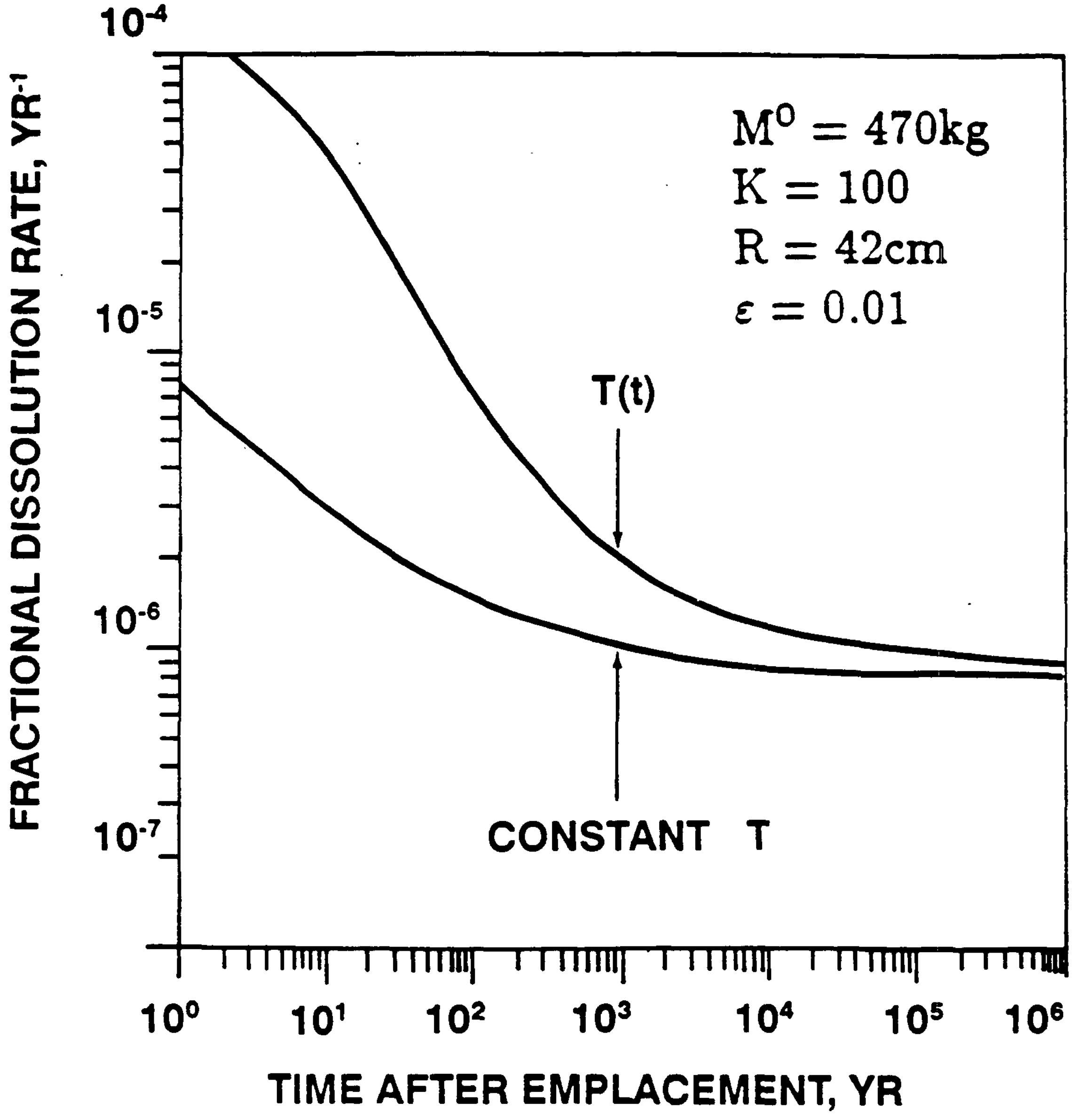
FRACTIONAL DISSOLUTION RATE FOR SILICA NORMALIZED TO INITIAL INVENTORY - EFFECT OF REPOSITORY HEATING



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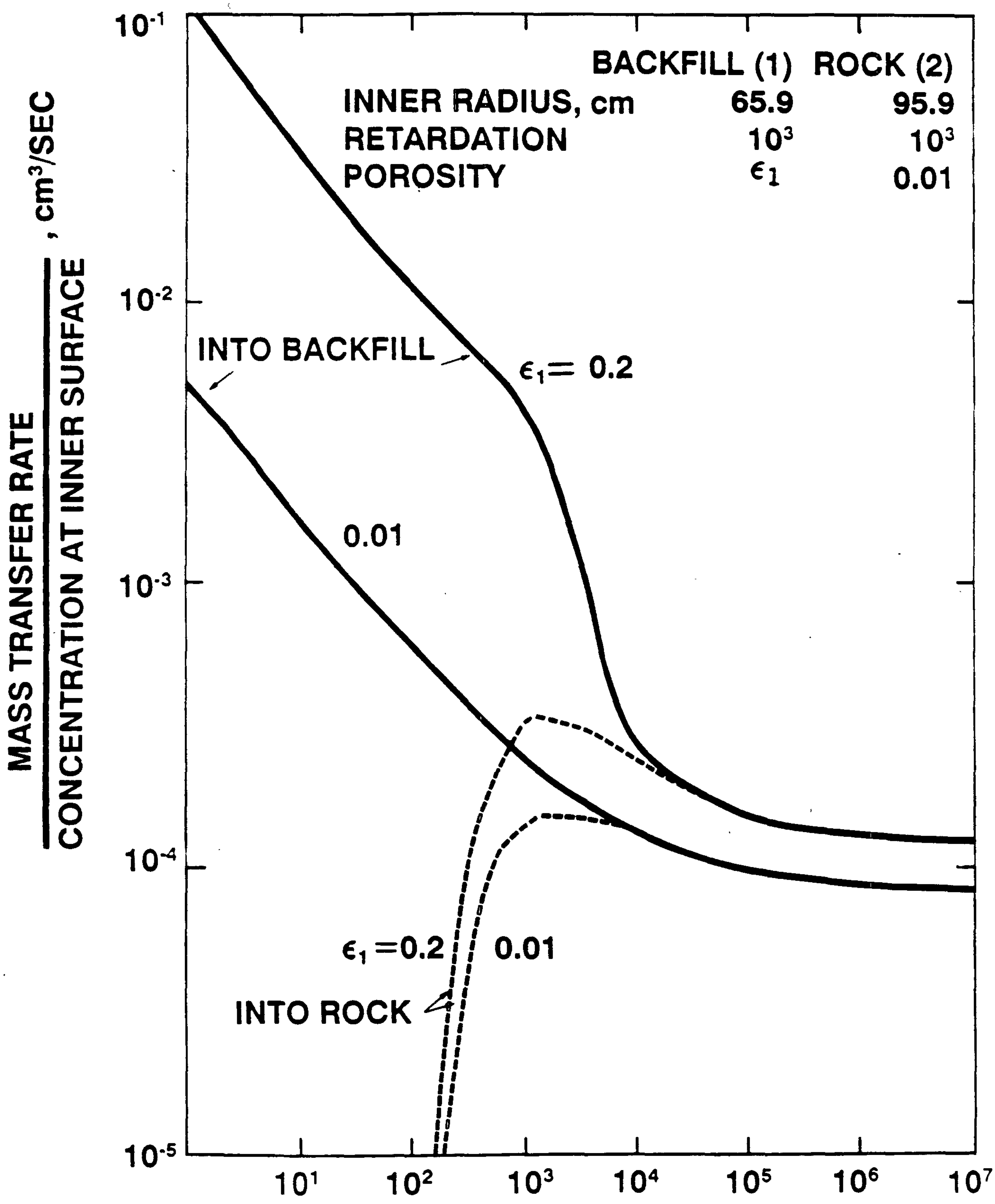
EFFECT OF BACKFILL POROSITY (ϵ)
(NO RADIOACTIVE DECAY)



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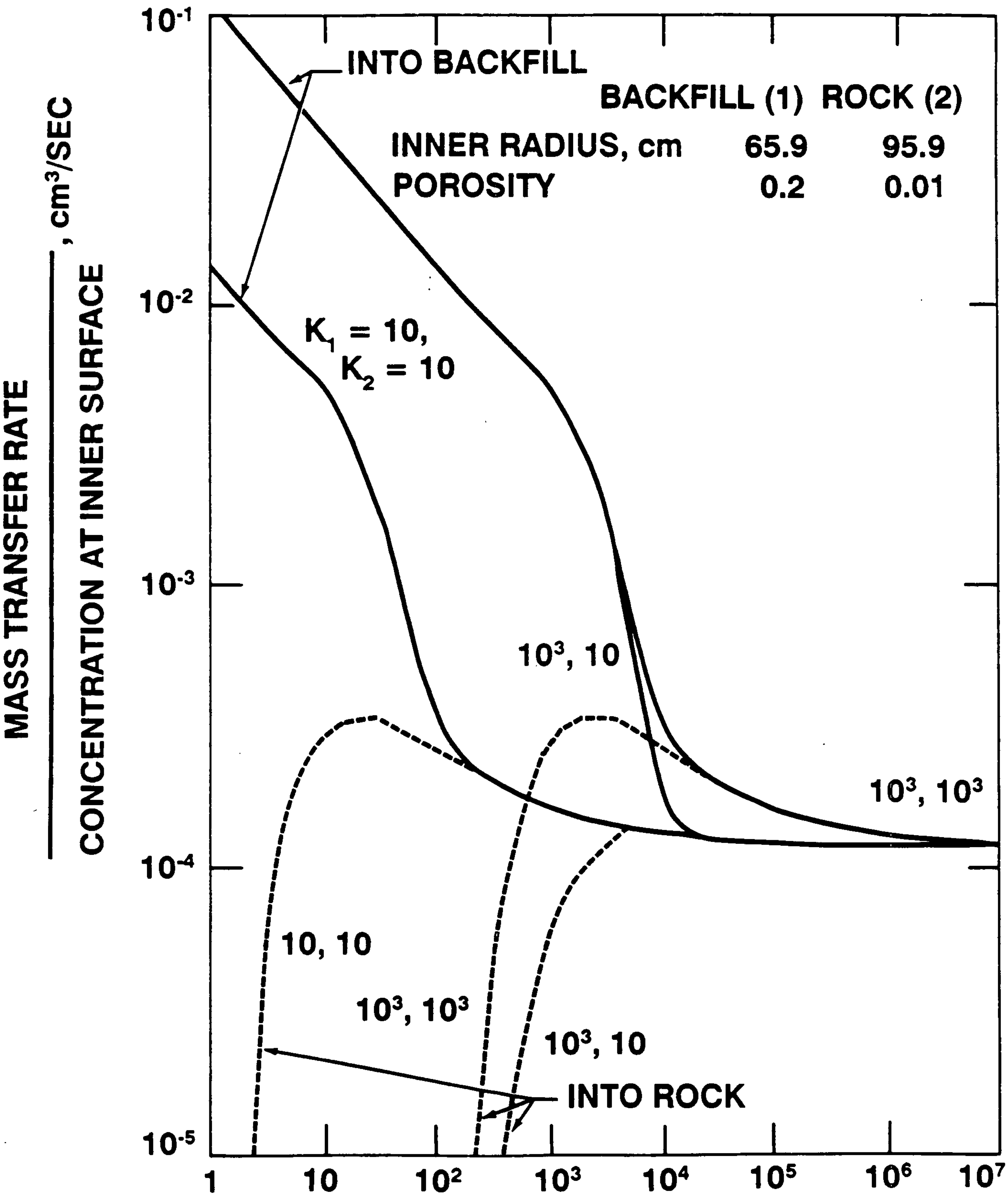
EFFECT OF RETARDATION (K) IN BACKFILL AND ROCK (NO RADIOACTIVE DECAY)



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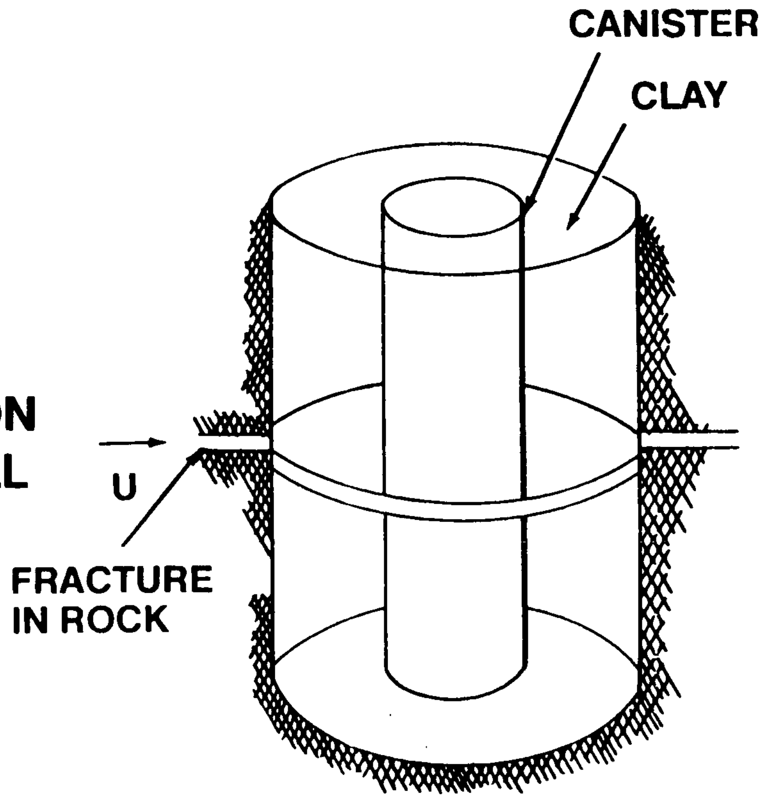
TRANSPORT OF RADIONUCLIDES IN THE BACKFILL SURROUNDING A WASTE FORM IN FISSURED ROCK

BACKGROUND

- IN MOST KINDS OF ROCK, THERE ARE NUMEROUS FRACTURES
- FRACTURES HAVE LARGER PERMEABILITY THAN ROCK

ASSUMPTION

- WATER-SATURATED BACKFILL
- NO CANISTER
- CONSTANT SPACING FRACTURE AND PERPENDICULAR TO WASTE FORM
- CONSTANT SURFACE CONCENTRATION
- NO GROUNDWATER FLOW IN BACKFILL
- COMPLETELY IMPERVIOUS ROCK



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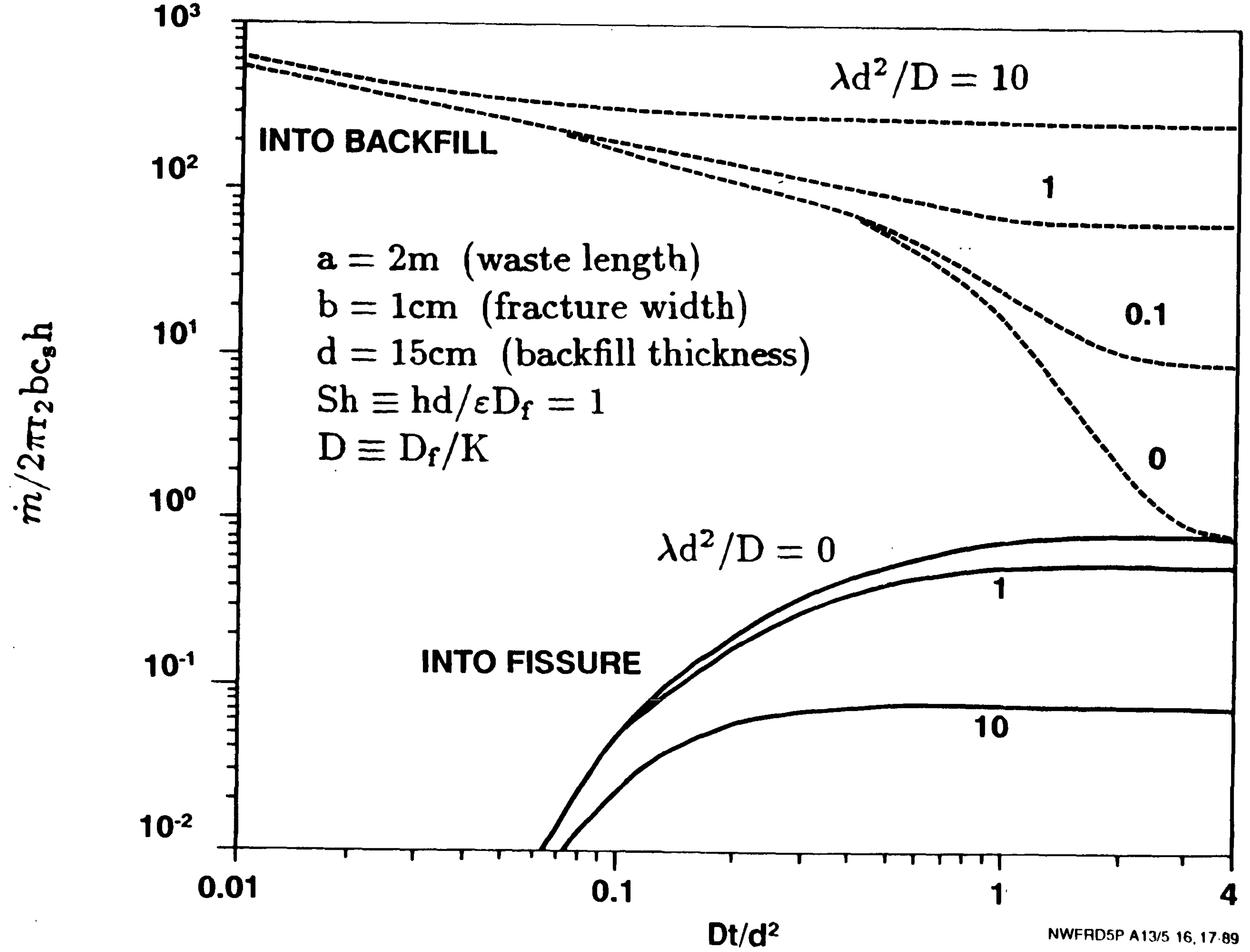
RELEASE INTO BACKFILL AND INTO FISSURED ROCK



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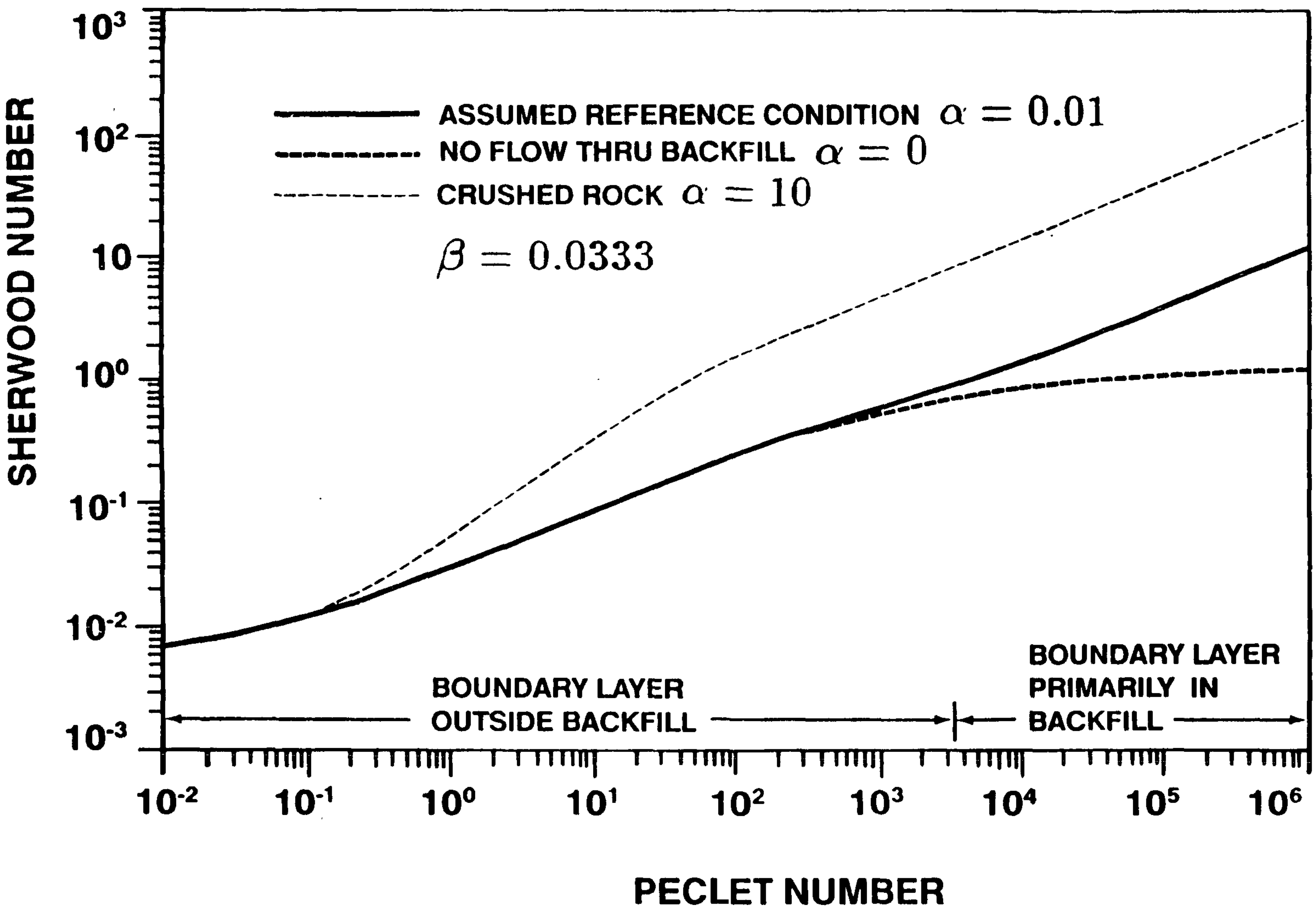
EFFECT OF FLOW THROUGH BACKFILL ON RELEASE RATE
(RELEASE RATE IS PROPORTIONAL TO SHERWOOD NUMBER)



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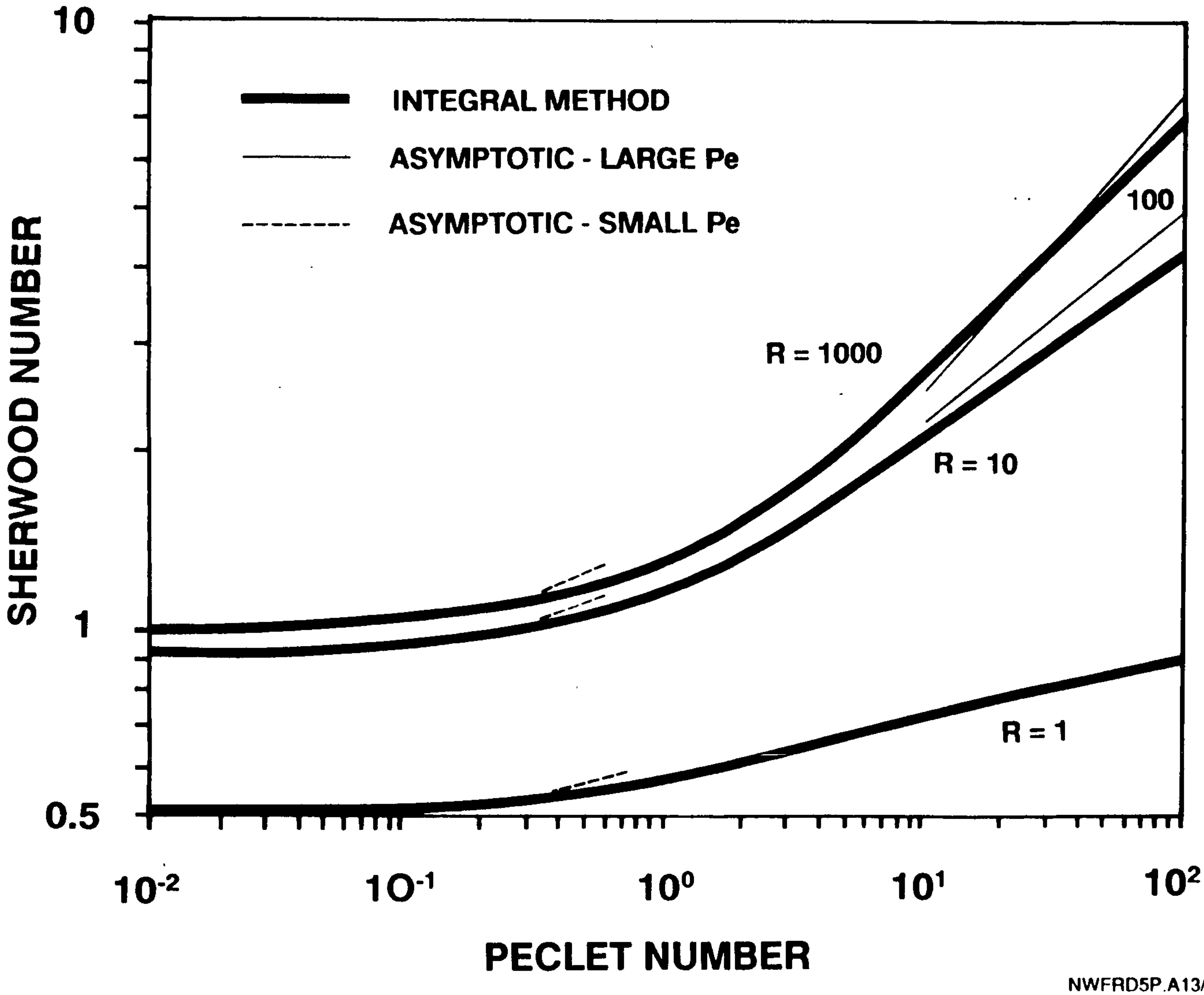
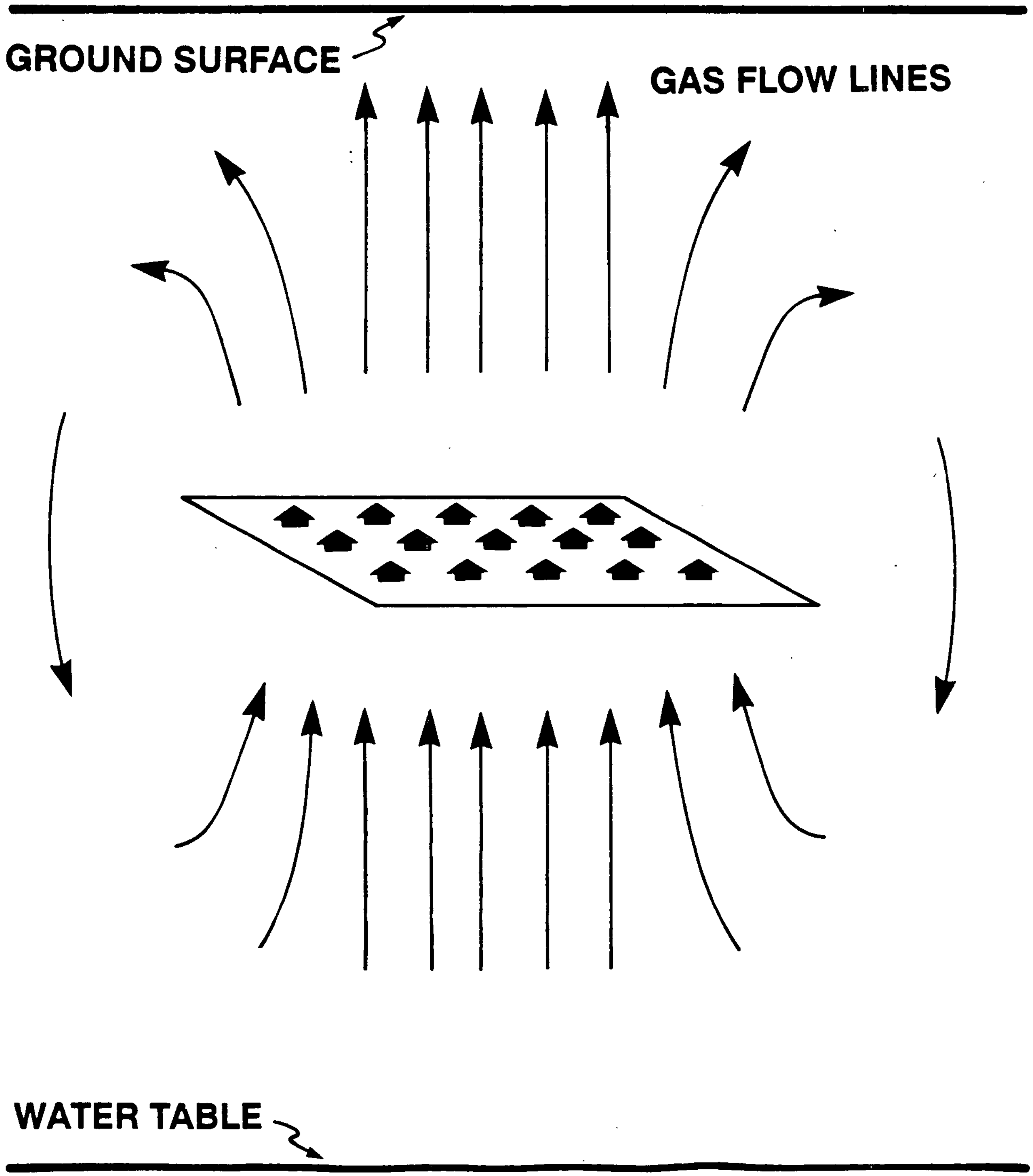
EFFECT OF FLOW RATE AND REACTION RATE ON RELEASE RATE (RELEASE RATE IS PROPORTIONAL TO THE SHERWOOD NUMBER)



NWFRD5P.A13/5-16, 17-89

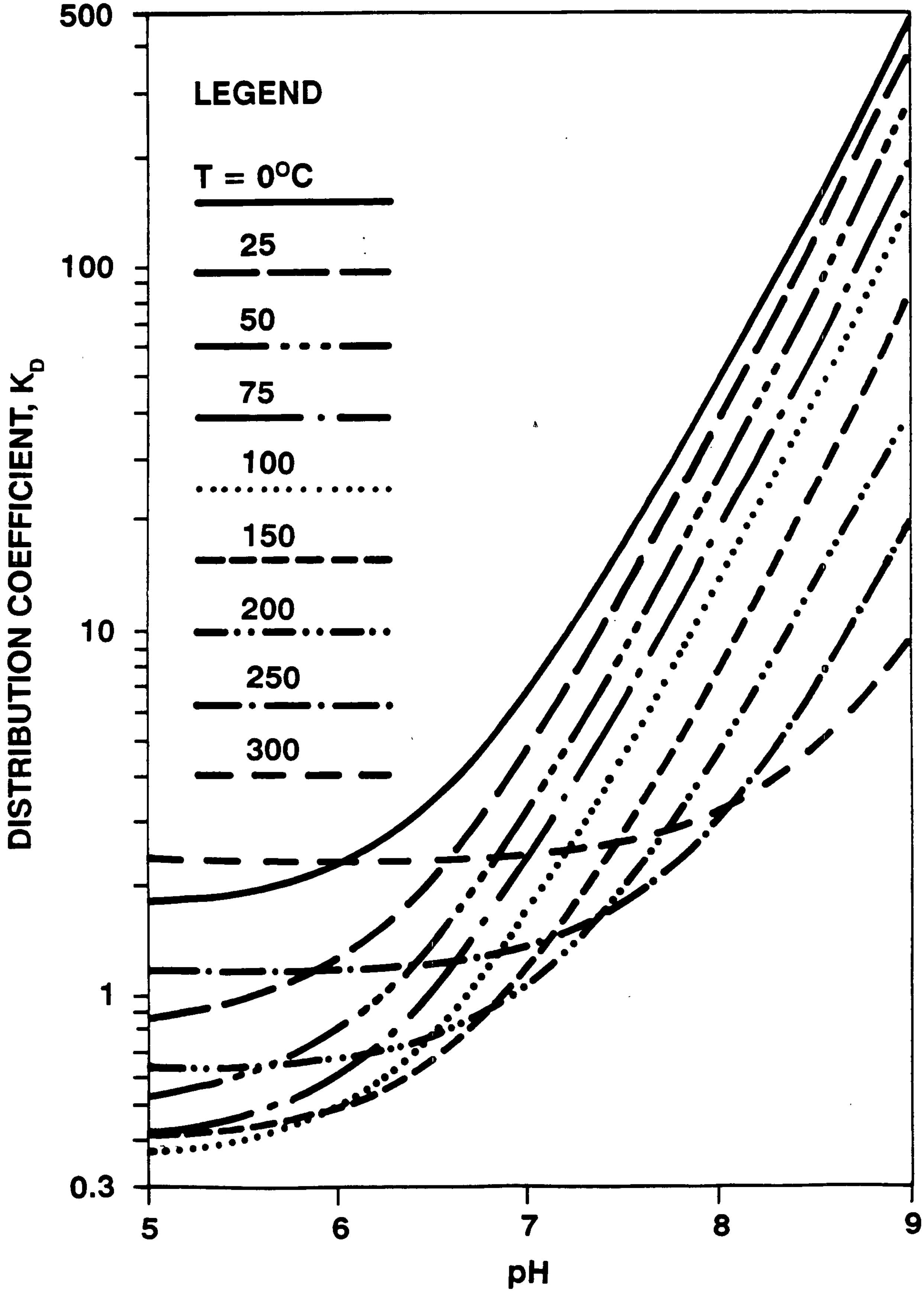
YUCCA MOUNTAIN HLW REPOSITORY
GAS FLOW FIELD

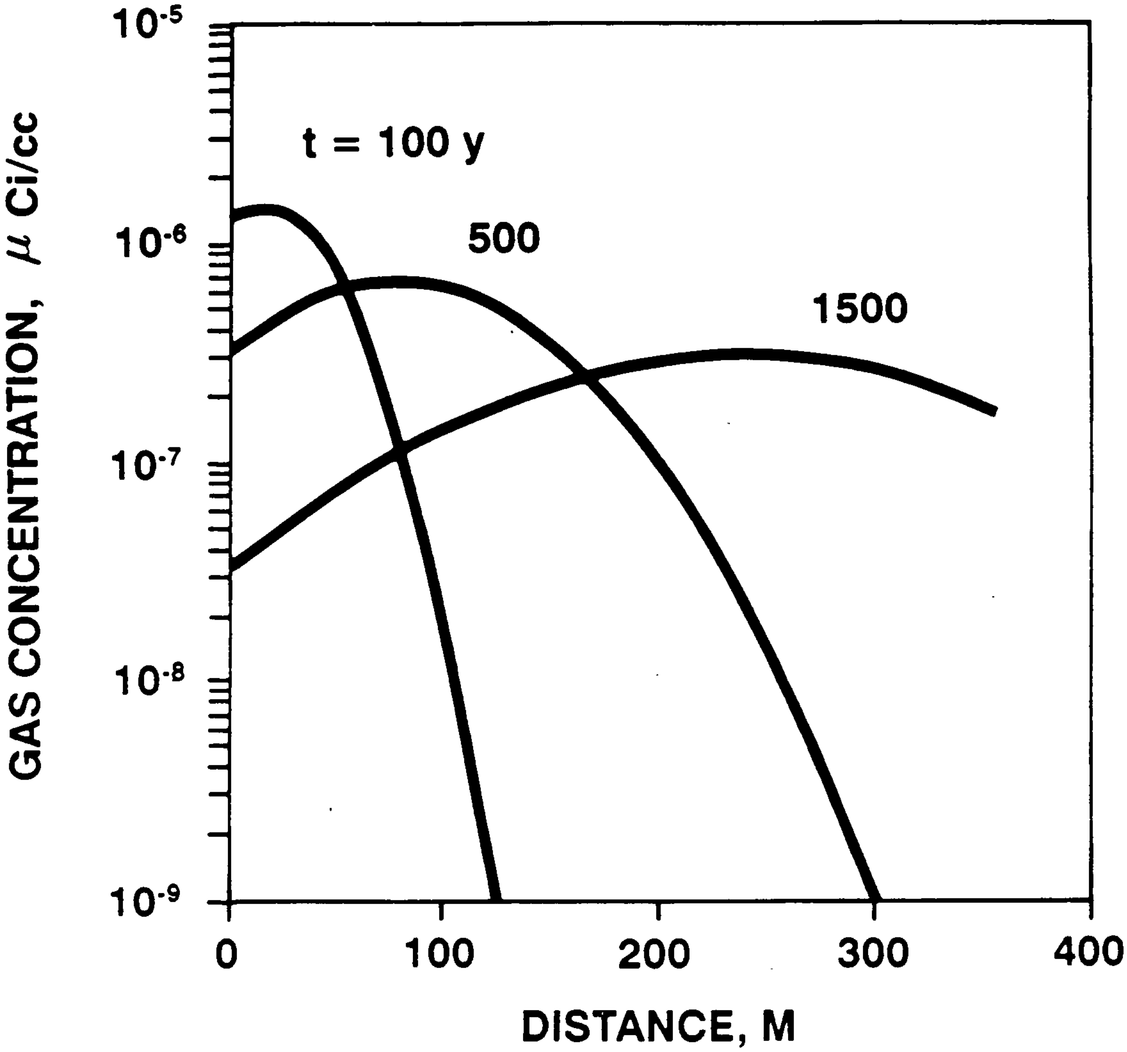


MODEL FEATURES

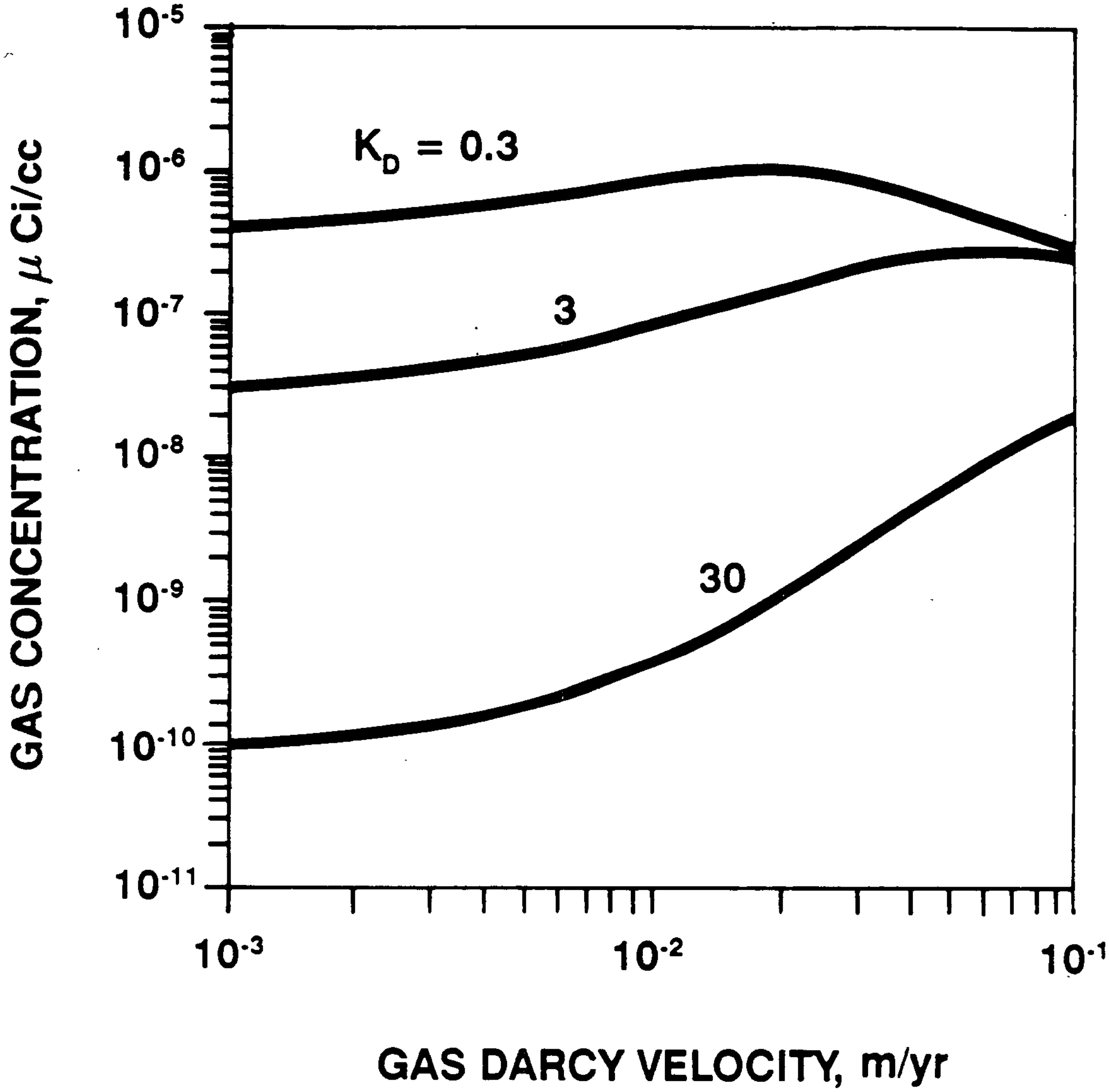
- ^{14}C IS RELEASED AS GASEOUS $^{14}CO_2$ AT THE REPOSITORY HORIZON
- $^{14}CO_2$ IS ADVECTED UPWARD THROUGH A FRACTURE
- SOME OF THE $^{14}CO_2$ DISSOLVES INTO THE PORE WATER OF THE ADJACENT WET-ROCK MATRIX
- EQUILIBRIUM IS MAINTAINED AT THE FRACTURE INTERFACE BETWEEN $^{14}CO_2$ IN THE GAS PHASE AND DISSOLVED ^{14}C IN THE LIQUID PHASE
- THE DISSOLVED ^{14}C DIFFUSES TRANSVERSLY IN THE WET-ROCK MATRIX

DISTRIBUTION COEFFICIENT FOR CO_2 ABSORPTION IN GROUND WATER

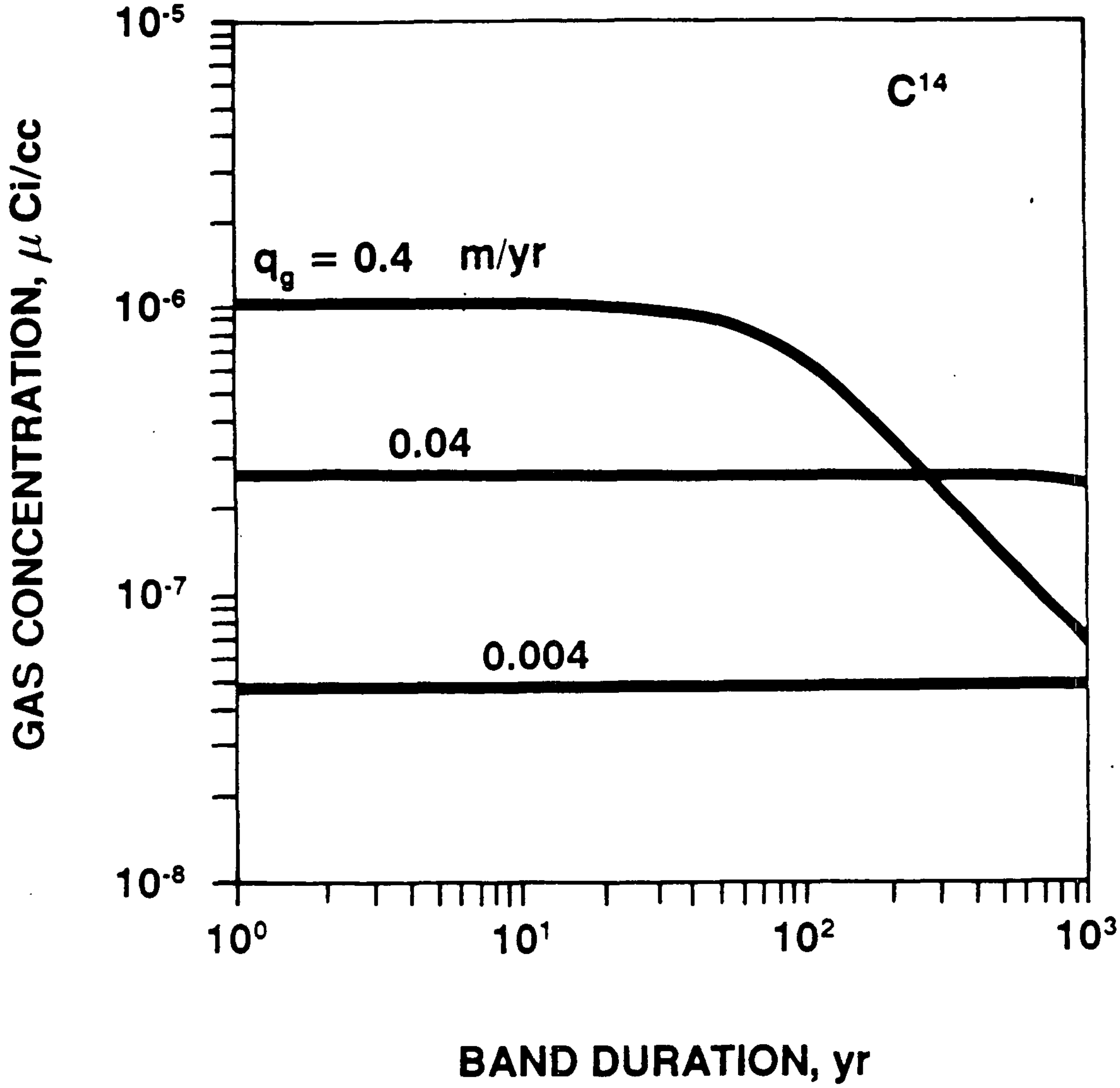




$^{14}CO_2$ CONCENTRATION VS. DISTANCE FOR IMPULSE RELEASE FROM INFINITE PLANE SOURCE (0.04 m/yr)

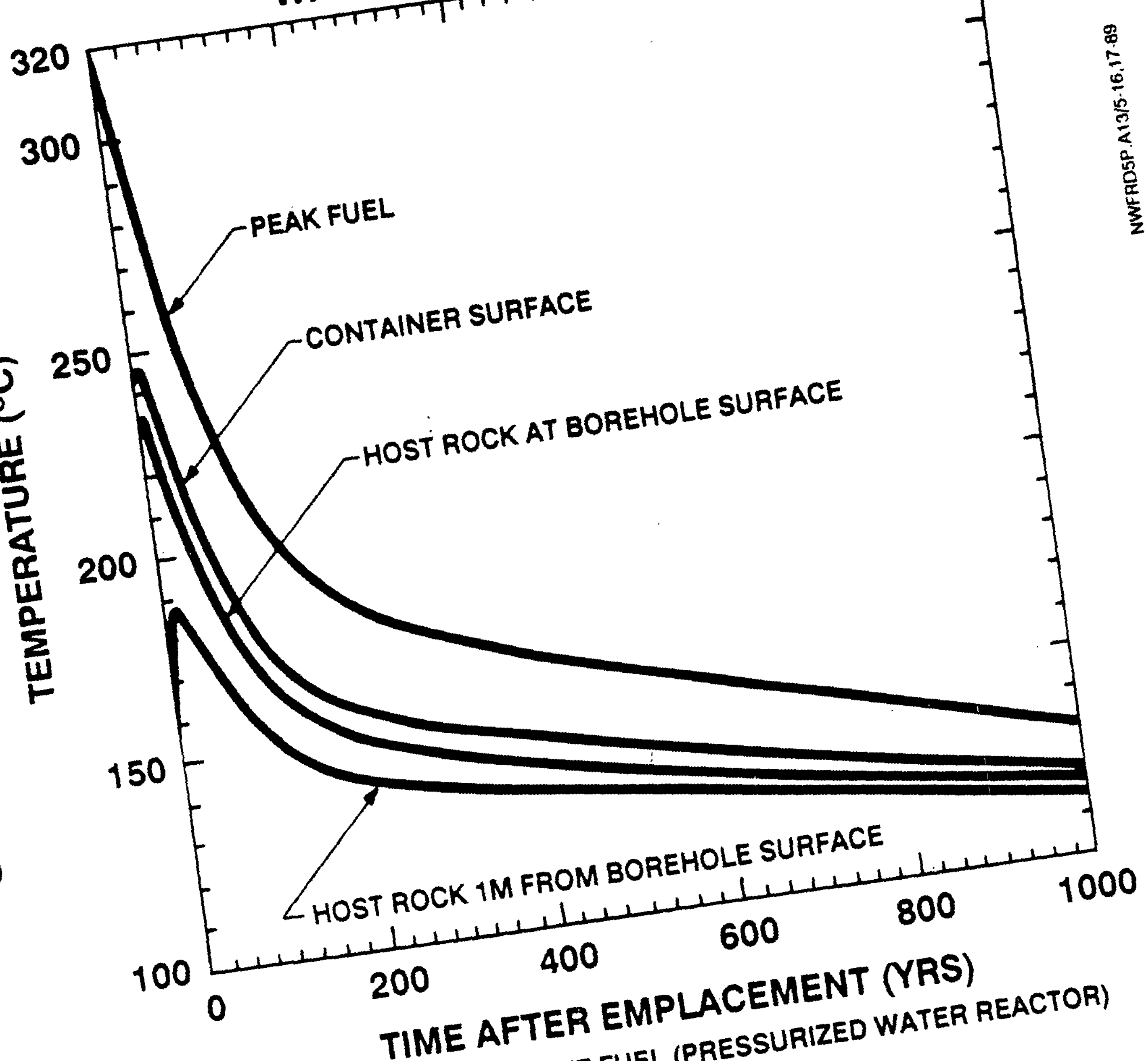


PEAK SURFACE CONCENTRATION OF $^{14}CO_2$ (Z = 350M) VS. GAS DARCY VELOCITY FOR BAND (1000 yr) RELEASE FROM INFINITE PLANE SOURCE



PEAK SURFACE CONCENTRATION OF $^{14}CO_2$ (Z = 350M) VS. BAND - RELEASE DURATION FOR INFINITE PLANE SOURCE

CALCULATED TEMPERATURE FOR REFERENCE WASTE PACKAGE IN TUFF



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WASTE FORM - SPENT FUEL (PRESSURIZED WATER REACTOR)

LOCAL POWER DENSITY - 57.0 KW/ACRE

AREAL POWER DENSITY - 48.4 KM/ACRE

AVERAGE PACKAGE POWER AT BURIAL - 3.3 KW
(10 YRS OUT OF REACTOR)

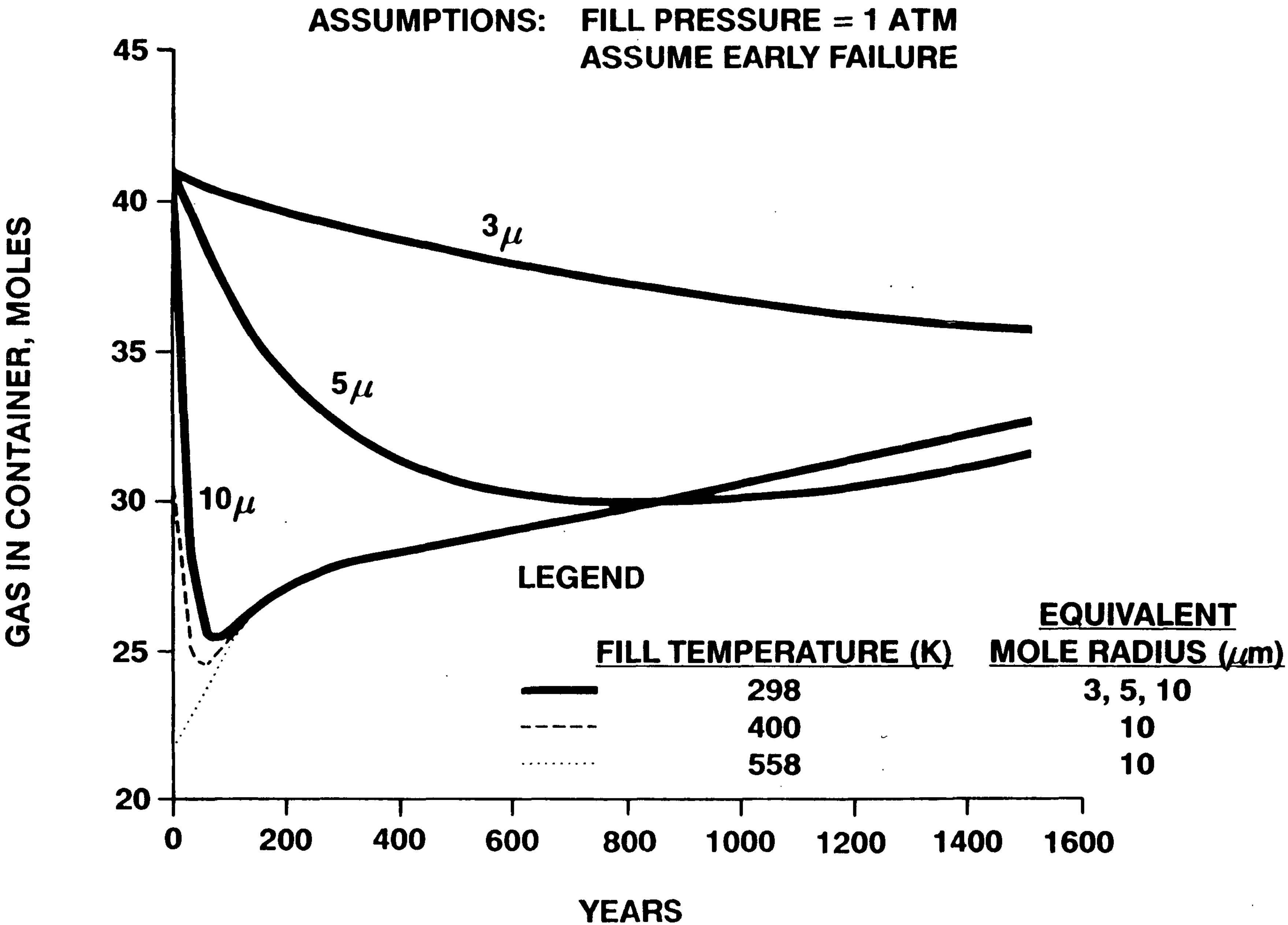
CONTAINER DIAMETER -0.7 M

PACKAGE SPACING - 5M

DRIFT SPACING - 46.86 M

DIRECTORY NO. - P57V3.3A
(DOE-SCP, 1988 p. 7-14)

GAS IN A WASTE CONTAINER, RESULT OF WASTE COOLING AND FLOW THROUGH PENETRATIONS



FURTHER WORK NEEDED

FOCUS

1. REFINE AND VALIDATE PRESENT PREDICTIVE CAPABILITY
   - METHODOLOGY
   - DATA BASE FOR PARAMETERS
2. EVALUATE GASEOUS RELEASES: $^{14}CO_2$, ^{3}H, ^{85}Kr, ^{129}I
3. ASSESS THE PREDICTION OF LOWER RELEASE RATES FROM MORE REALISTIC MODELS
4. EVALUATE ADDITIONAL PHENOMENA THAT CAN AFFECT RELEASE RATES

SPECIFIC EXAMPLES OF FURTHER WORK NEEDED

1. REFINE AND VALIDATE PRESENT PREDICTIVE CAPABILITY

- DEVELOP PROGRAM-WIDE UNDERSTANDING OF PRESENT CAPABILITY AND OF DATA NEEDS VIA TIG'S NEW TEST PROBLEMS
- COMPLETE DOCUMENTATION OF PRESENT CAPABILITY
- APPLY ADDITIONAL SUBMODELS ALREADY DEVELOPED
- REFINE DATA AND ANALYSES ON EFFECTIVE SATURATION CONCENTRATIONS, INCLUDING EFFECT OF AIR INFLOW THROUGH FAILED CONTAINERS
- MEASURE LIQUID DIFFUSION COEFFICIENTS AND CONNECTED POROSITY IN TUFF
- PERFORM EXPERIMENTS TO VALIDATE THE THEORY UNDERLYING THE PREDICTIVE MODELS

SPECIFIC EXAMPLES OF FURTHER WORK NEEDED

2. EVALUATE GASEOUS RELEASES

- DETERMINE THE TIME-DEPENDENT SOURCE AND AMOUNT OF $^{14}CO_2$, ^{3}H, ^{85}Kr, ^{129}I THAT CAN BE MOBILIZED WITHIN A FAILED WASTE PACKAGE AND THE RATE OF ESCAPE THROUGH PENETRATIONS

- EVALUATE THE SPACE-TIME-DEPENDENT RETARDATION COEFFICIENT FOR CARBON DIOXIDE, AS AFFECTED BY TEMPERATURE, pH, LOCAL MOISTURE CONTENT IN TUFF, CALCITE, AND GROUND-WATER EVAPORATION

- EVALUATE THE SPACE-TIME-DEPENDENT FLOW RATE OF AIR IN THE HEATED REPOSITORY

- DETERMINE THE EXTENT TO WHICH THE PEAK CONCENTRATIONS OF GASEOUS EFFLUENTS AT THE SUBSURFACE ARE AFFECTED BY THEIR RATE OF RELEASE AT THE REPOSITORY HORIZON

SPECIFIC EXAMPLES OF FURTHER WORK NEEDED

3. INVESTIGATE MORE REALISTIC MODELS THAT ARE EXPECTED TO PREDICT LOWER RELEASE RATES TO GROUND WATER

   - DEVELOP A MODEL FOR THE TIME OF CONTAINER FAILURE BY LOCALIZED PENETRATIONS AND THE SIZE, GEOMETRY, AND GROWTH OF THOSE PENETRATIONS

   - DETRMINE THE FLOW OF GROUND WATER THROUGH THE SMALL PENETRATIONS IN A FAILED CONTAINER

   - DETERMINE THE RATE OF DIFFUSION AND CONVECTION OF DIS-SOLVED RADIONUCLIDES OUT OF CONTAINER PENETRATIONS

   - DETERMINE THE EFFECT OF TRANSPORT BARRIERS DUE TO SMALL PENETRATIONS IN DEFECTIVE FUEL CLADDING

   - DETERMINE THE EFFECT OF UNCONNECTED POROSITY IN UNSATURATED TUFF ON DIFFUSIVE TRANSPORT

   - DETERMINE THE TRANSPORT THROUGH RUBBLE IN THE CONTAINER-ROCK ANNULUS

SPECIFIC EXAMPLES OF FURTHER WORK NEEDED

4. EVALUATE THE EFFECT OF ADDITIONAL PHENOMENA THAT CAN AFFECT RELEASE RATES

- AIR INLEAKAGE THROUGH FAILED CONTAINERS
  - EFFECT ON SATURATION CONCENTRATIONS
  - OXIDATION OF ZIRCALOY CLADDING
  - OXIDATION OF URANIUM DIOXIDE
  - MOBILIZATION OF GASEOUS SPECIES

- ALPHA RADIOLYSIS
  - CAN RESULT IN HIGHER OXIDATIONS STATES AND INCREASED SATURATION CONCENTRATION
  - A REDOX FRONT NEAR THE WASTE SURFACE AND AN INCREASED CONCENTRATION GRADIENT AT THE WASTE SURFACE CAN INCREASE RELEASE RATE INTO GROUND WATER

- DIFFUSIVE-ADVECTIVE MASS TRANSFER FROM WASTE SOLID TO WATER INSIDE A WASTE CONTAINER
  - POTENTIALLY IMPORTANT IF VOID SPACE INSIDE CONTAINER IS FILLED WITH LOW-POROSITY MATERIAL