ATTACHMENT 15

YUCCA
MOUNTAIN
PROJECT

Studies

Model Development for Crevice Corrosion & Pitting of Inner Barrier

Presented to:
DOE/NRC Technical Exchange on
Total System Performance Assessment
Las Vegas, Nevada

Presented by:
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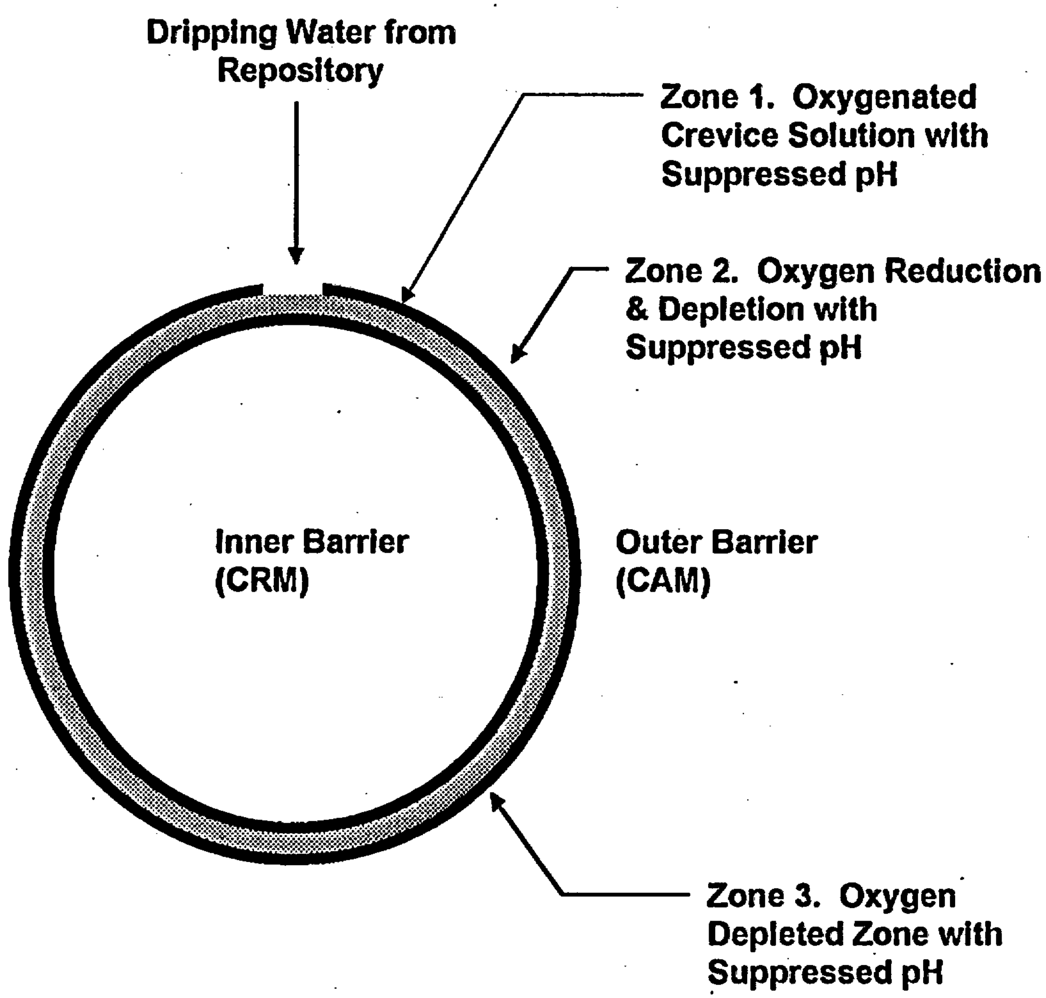
November 6, 1997

U.S. Department of Energy
Office of Civilian Radioactive
Waste Management

Conceptual representation of WP under attack



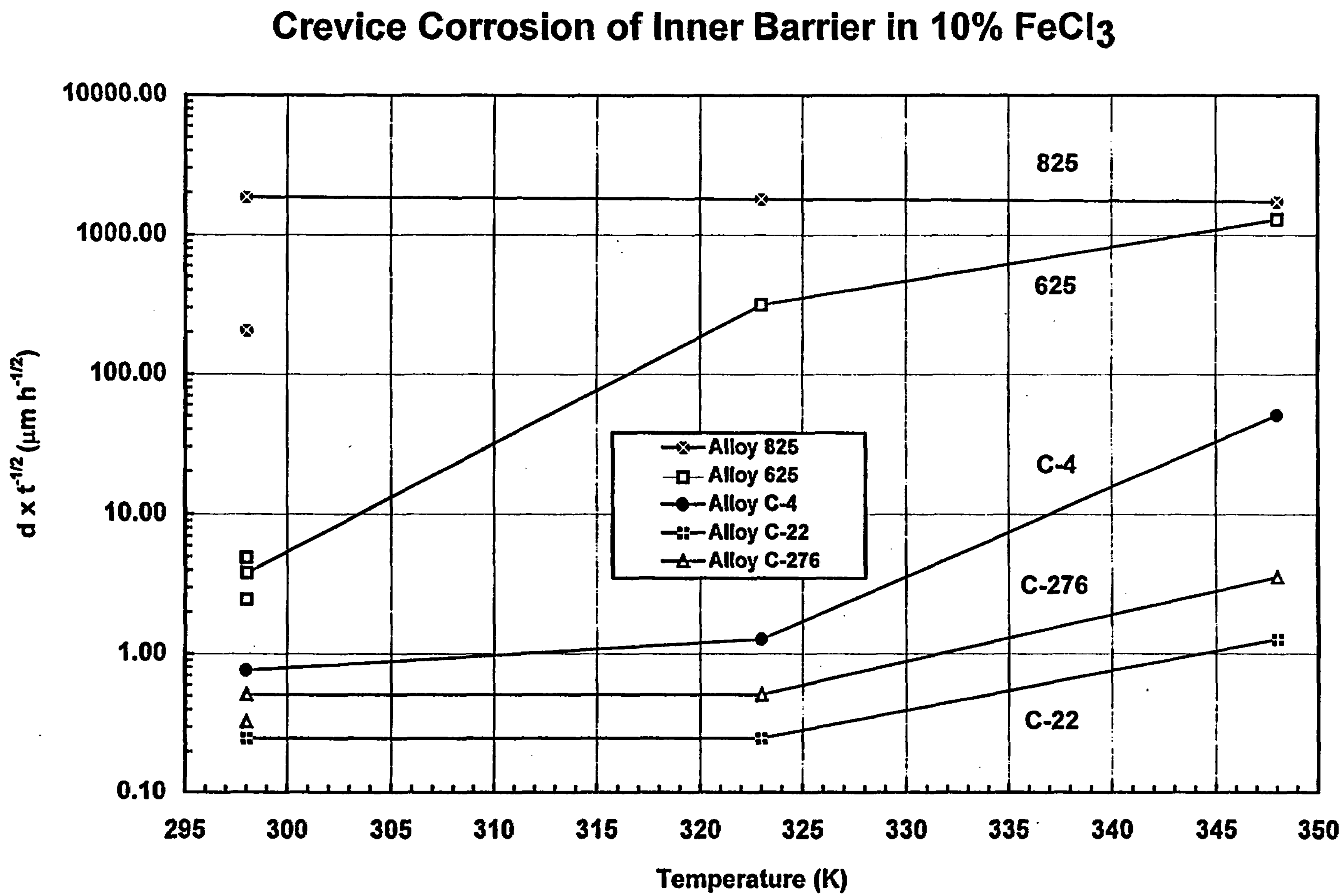
J.C. Farmer, LLNL, October 1997

Anticipated conditions in three zones

- Oxygen concentration
  - Zone 1: O_2 same as NFE
  - Zone 2: gradient due to simultaneous diffusion & reaction
  - Zone 3: depleted
- Hydrogen & chloride ion concentrations
  - Zone 1: pH & Cl^- should be about the same as NFE
  - Zone 2: suppressed pH & enhanced Cl^- due to hydrolysis
  - Zone 3: suppressed pH & enhanced Cl^- due to hydrolysis
- Dominant electrochemical reactions
  - Zone 1: O_2 reduction & anodic dissolution of CAM or CRM
  - Zone 2: O_2 & H^+ reduction & anodic dissolution of CAM or CRM
  - Zone 3: H^+ reduction & anodic dissolution of CAM or CRM

Observed crevice corrosion of Alloy 625

- The crevice corrosion of Alloy 625 has been documented
  - Photograph of Alloy 625 in chlorinated ASTM artificial sea water
    - R. S. Lillard, J. R. Scully, Modeling of the Factors Contributing to the Initiation and Propagation of the Crevice Corrosion of Alloy 625, J. Electrochem. Soc., Vol. 141, No. 11, 1994, pp. 3006-3015.
  - Penetration rate data for $FeCl_3$ solutions (simulated crevice)
    - Haynes International, Inc., Hastelloy Alloy C-276, Haynes Product Brochure H-2002B, Haynes International, 1987.
    - A. I. Asphahani, Corrosion Resistance of High Performance Alloys, Materials Performance, Vol. 19, No. 12, 1980, pp. 33-43.
- No significant attack observed in less severe conditions
  - Concentrated electrolytes without $FeCl_3$ (no CAM corrosion)
    - LLNL, 6-month exposure test, concentrated J-13, August 1997.
    - H. P. Hack, Crevice Corrosion Behavior of Molybdenum-Containing Stainless Steel in Seawater, Materials Performance Vol. 22, No. 6, 1983, pp. 24-30.


Crevice Corrosion of Inner Barrier in 10% FeCl3
d x t^-1/2 (µm h^-1/2)
10000.00
1000.00
100.00
10.00
1.00
0.10
295
300
305
310
315
320
325
330
335
340
345
350
Temperature (K)
825
625
C-4
C-276
C-22
Alloy 825
Alloy 625
Alloy C-4
Alloy C-22
Alloy C-276

Fi[illegible] 2

Semi-Empirical Model: Crevice Corrosion of Inner Barrier in 10% $FeCl_3$

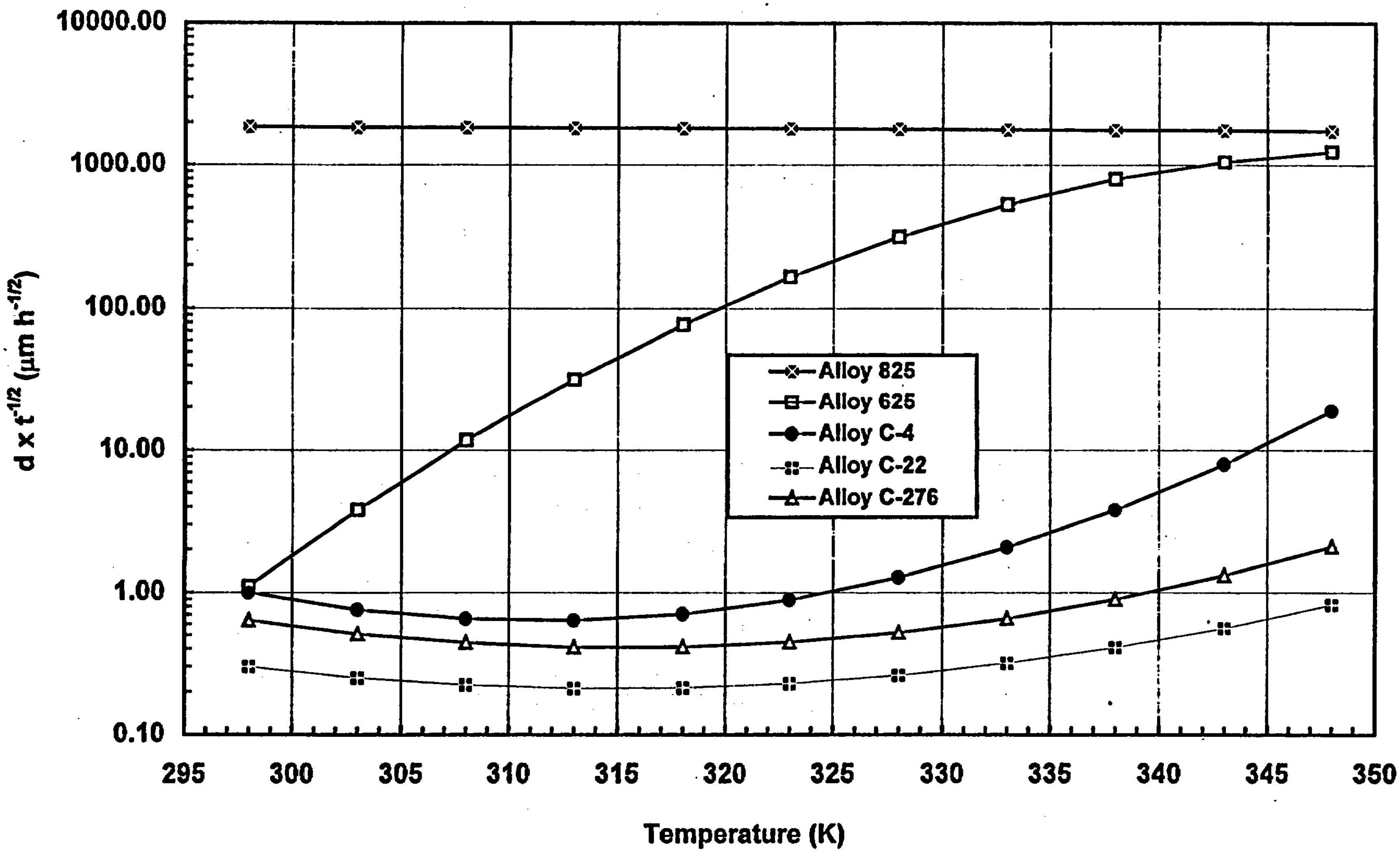


Figure 3

Crevice Corrosion of Inner Barrier in $FeCl_3$ at 80° Centigrade

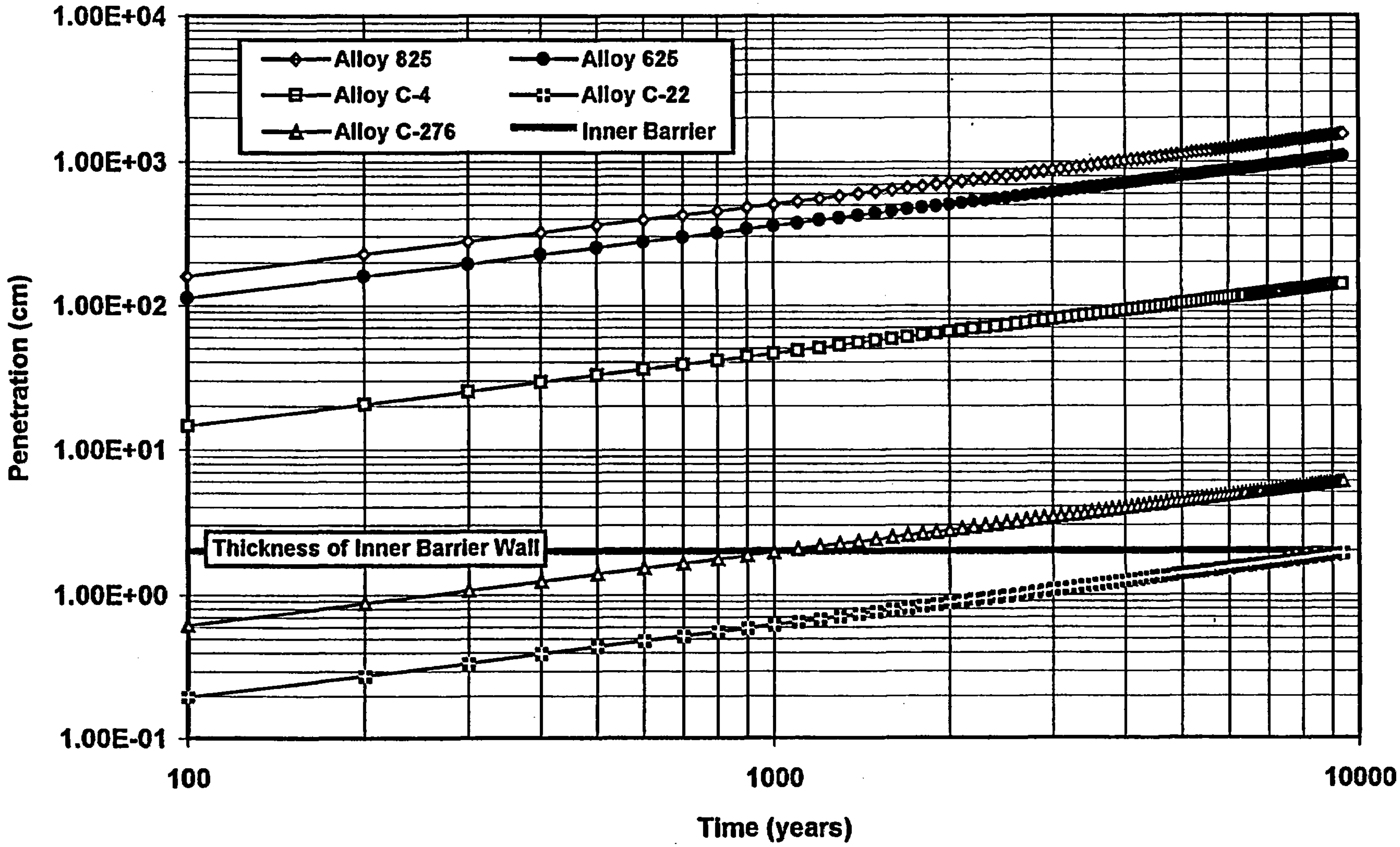


Fig. 4

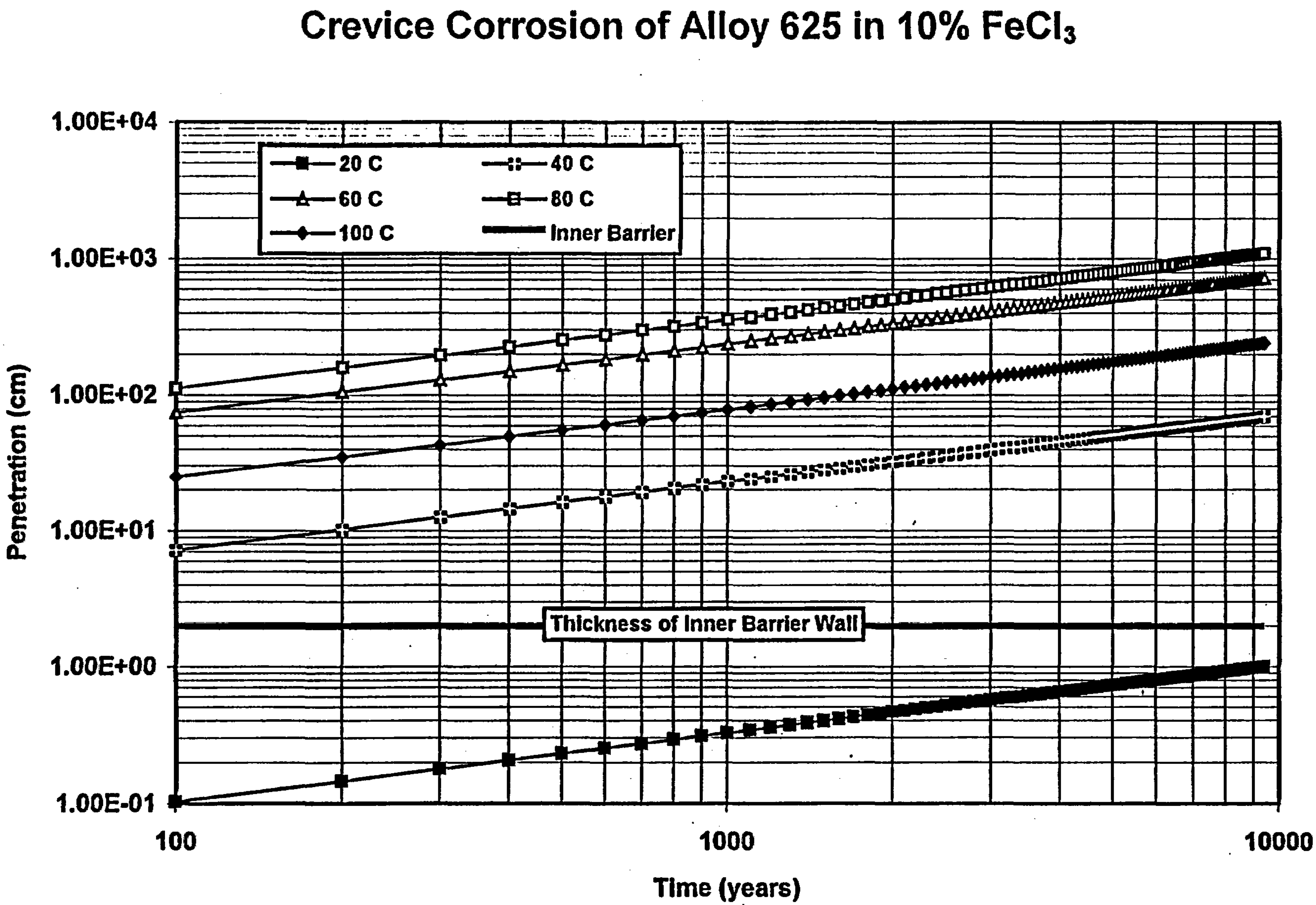
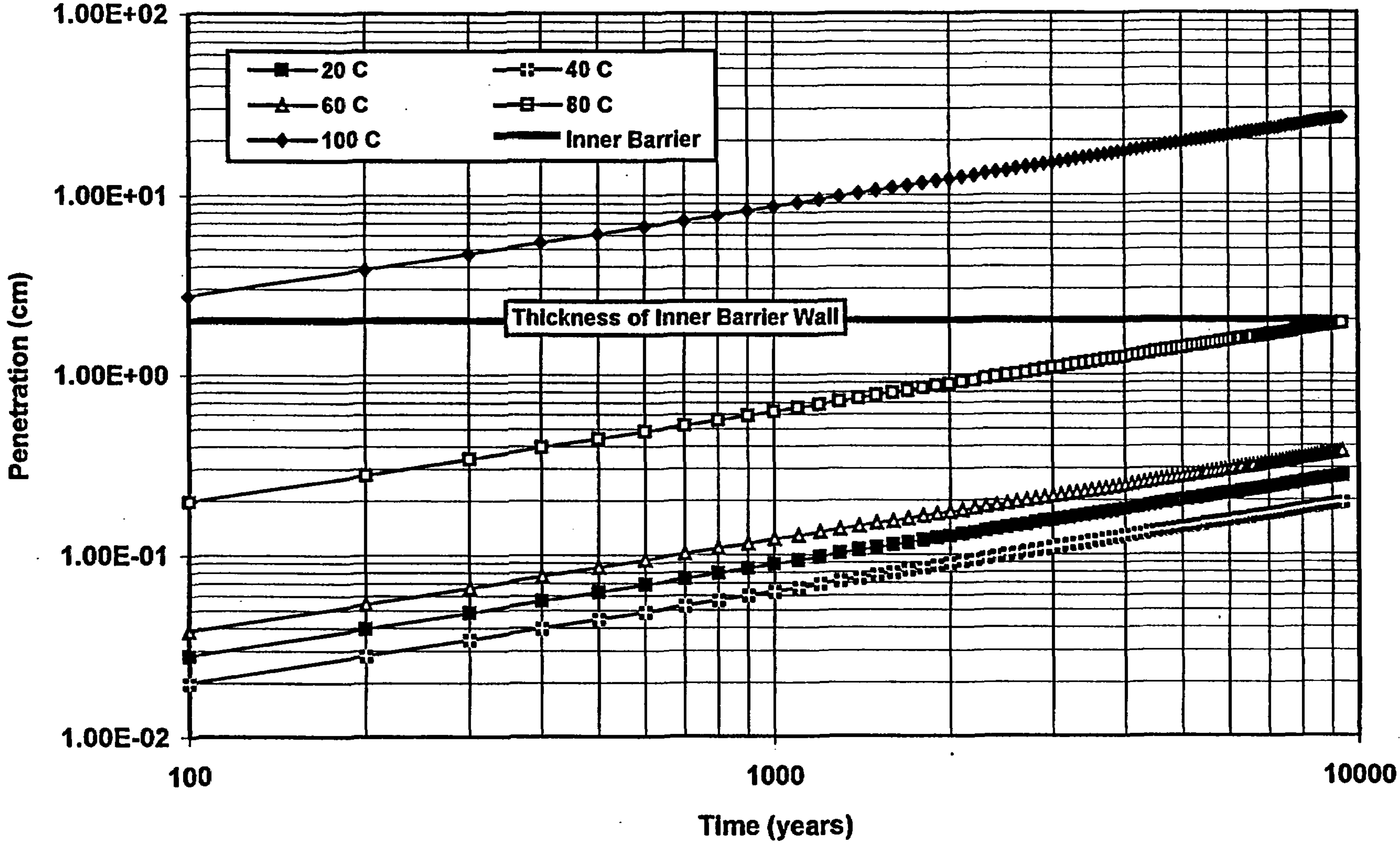

Crevice Corrosion of Alloy 625 in 10% FeCl3
20 C
40 C
60 C
80 C
100 C
Inner Barrier
Thickness of Inner Barrier Wall
1.00E+04
1.00E+03
1.00E+02
1.00E+01
1.00E+00
1.00E-01
Penetration (cm)
100
1000
10000
Time (years)

Figure 5

Crevice Corrosion of Alloy C-22 in 10% $FeCl_3$



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Crevice corrosion should be accounted for by TSPA

- Crevices will be formed
  - Between waste package and supports
  - Between CAM and CRM
  - Beneath dust, scale and biofilms
- The crevice environment will be more severe than the NFE
  - Suppression of pH due to the accumulation of H^+ from the hydrolysis of dissolved metal
  - Field-driven electromigration of Cl^- (and other anions) into crevice must occur to balance cationic charge associated with H^+
- The crevice environment sets the stage for other modes of attack
  - General corrosion
  - Pitting (initiation & propagation)
  - Stress corrosion cracking (initiation & propagation)
- The development of an adequate crevice corrosion model is prudent

Crevice corrosion models

- Crevice corrosion was categorized on the basis of concentration-cell type by France
  - Metal ion
  - Differential aeration
  - Active-passive
  - Hydrogen ion
  - Neutral salt
  - Inhibitor
- Numerical model by Oldfield & Sutton divided crevice corrosion phenomena into four stages
  - Depletion of oxygen in crevice
  - Increase in acidity and chloride concentration in crevice
  - Permanent breakdown of the passive film & active corrosion
  - Propagation of crevice corrosion

Crevice corrosion models (cont'd.)

- Model developed by Pickering & Xu
  - Applicable to cases involving active-passive transition
  - Calculates current from measured potential distribution
  - Used to establish critical distance for depassivation (d_c)
    - Passive walls for ($x < d_c$)
    - Active corrosion for ($x > d_c$)
- Model developed by Lillard & Scully
  - Based on linear network theory (an equivalent circuit model)
  - Used to interpret potential & current distributions
  - Applied to the observed crevice corrosion of Alloy 625
- Model developed by LLNL
  - Concentration profiles of reactive and non-reactive species
  - Current and potential distributions (limited by local E_{mix})
  - Hydrolysis of Fe, Ni, Cr and Mo

LLNL crevice corrosion model

- **Nernst-Planck equation (Newman; Bard & Faulkner)**

$$\overline{N}_i = -z_i u_i F c_i \overline{\nabla}\Phi - D_i \overline{\nabla} c_i + \overline{v} c_i$$

- **Transient concentrations**

$$\frac{\partial c_i}{\partial t} = -\overline{\nabla} \cdot \overline{N}_i + R_i$$

- **Current density**

$$\overline{i} = -F^2 \overline{\nabla}\Phi \sum_i z_i^2 u_i c_i - F \sum_i z_i D_i \overline{\nabla} c_i$$

- **One-dimensional transport without convection**

$$N_{i,x} = -z_i u_i F c_i \frac{\partial \Phi}{\partial x} - D_i \frac{\partial c_i}{\partial x}$$

$$i_x = -\kappa_x \frac{\partial \Phi}{\partial x} - F \sum_i z_i D_i \frac{\partial c_i}{\partial x} \qquad \kappa_x = -F \sum_i z_i^2 u_i c_i$$

- **Strong supporting electrolyte - electromigration terms unimportant**

LLNL crevice corrosion model (cont'd.)

- **Application of the Explicit Method - concentration profile**

$$C_{m,n+1} = A\left(C_{m+1,n} + C_{m-1,n}\right) + (1-2A)C_{m,n} + (\Delta t)R_{m,n}$$

Truncation error: $T_{m,n} \le \frac{A(6A-1)}{12} Mh^4$

Modulus: $A = \frac{D(\Delta t)}{(\Delta x)^2}$

Boundary conditions: $C_{1,n} = 0$ *and* $C_{m+1,n} = C_{m-1,n}$

- **Application of the Crank-Nicholson Method - concentration profile**

$$C_{m,n+1} = \frac{A}{2(1+A)}\left(C_{m+1,n+1} + C_{m-1,n+1}\right) + \frac{(1-A)}{(1+A)}C_{m,n} + \frac{A}{2(1+A)}\left(C_{m+1,n} + C_{m-1,n}\right) + \frac{(\Delta t)}{(1+A)}R_{m,n}$$

Truncation error: $T_{m,n} \le \frac{A}{12} Mh^4$

Modulus: $A = \frac{D(\Delta t)}{(\Delta x)^2}$

Boundary conditions: $C_{1,n} = 0$ *and* $C_{m+1,n} = C_{m-1,n}$

Finite Element Model of Crevice - Explicit Method

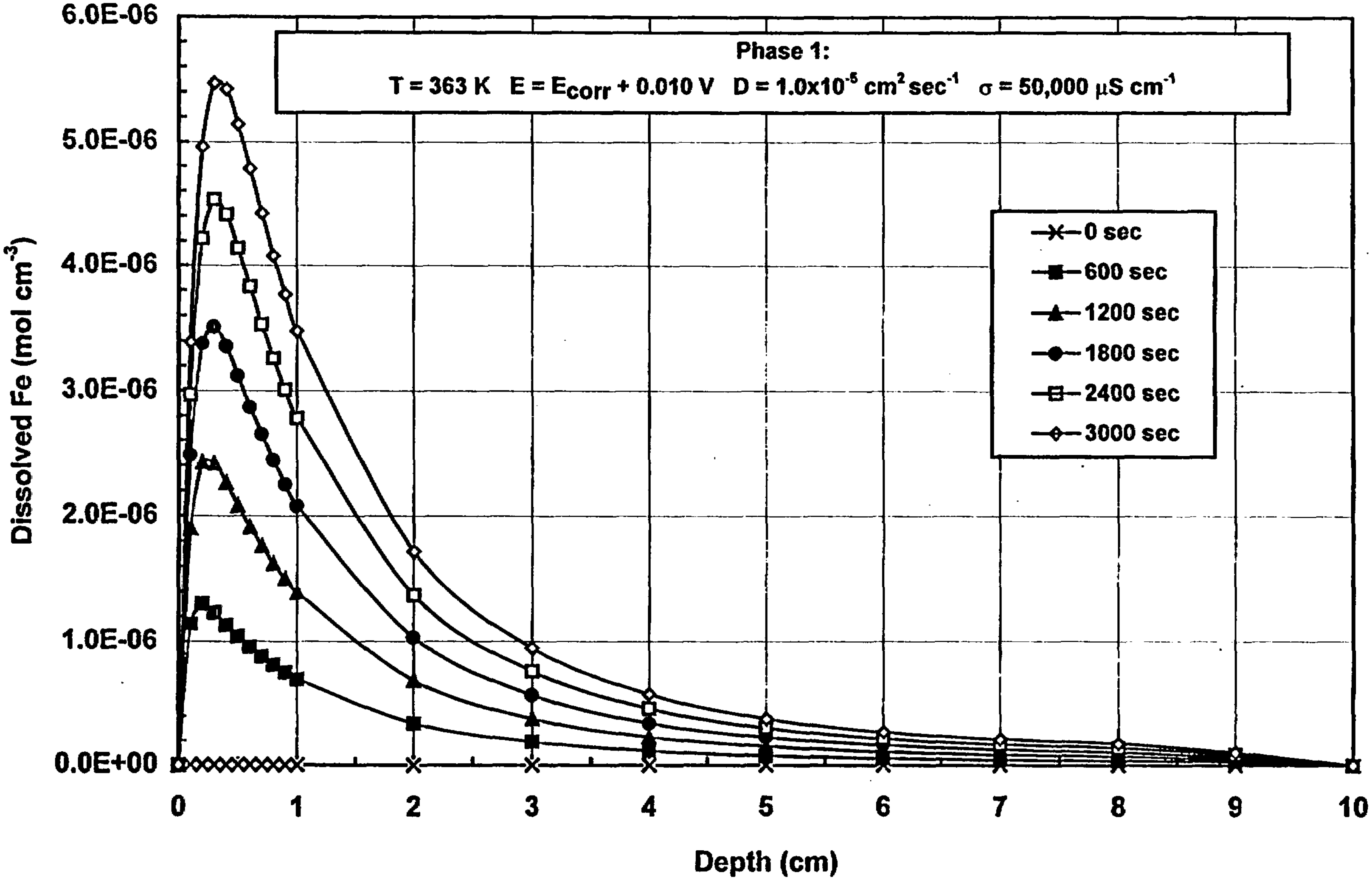


Figure 7a

Finite Element Model of Crevice - Crank-Nicholson Method

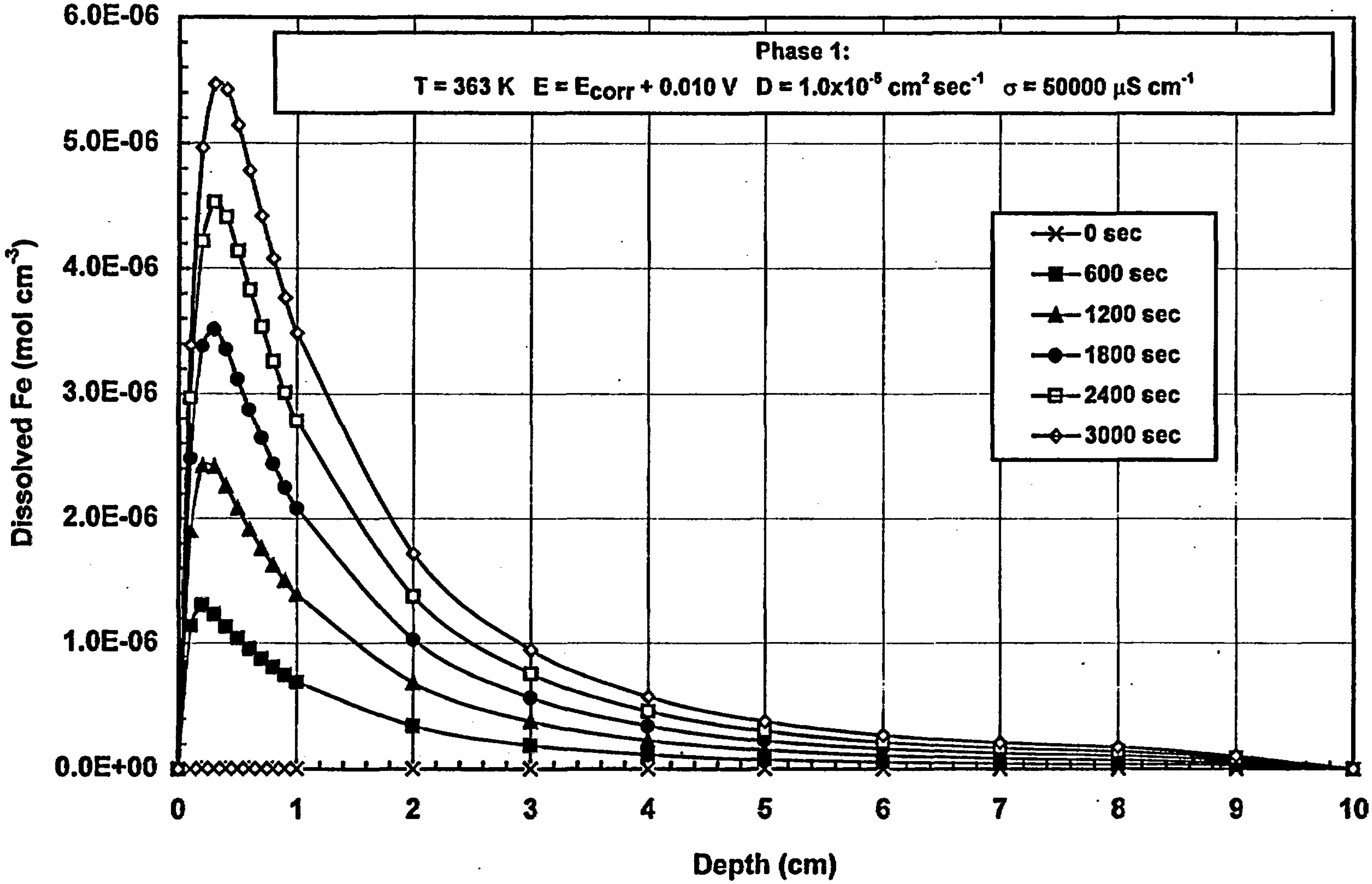


Figure 7b

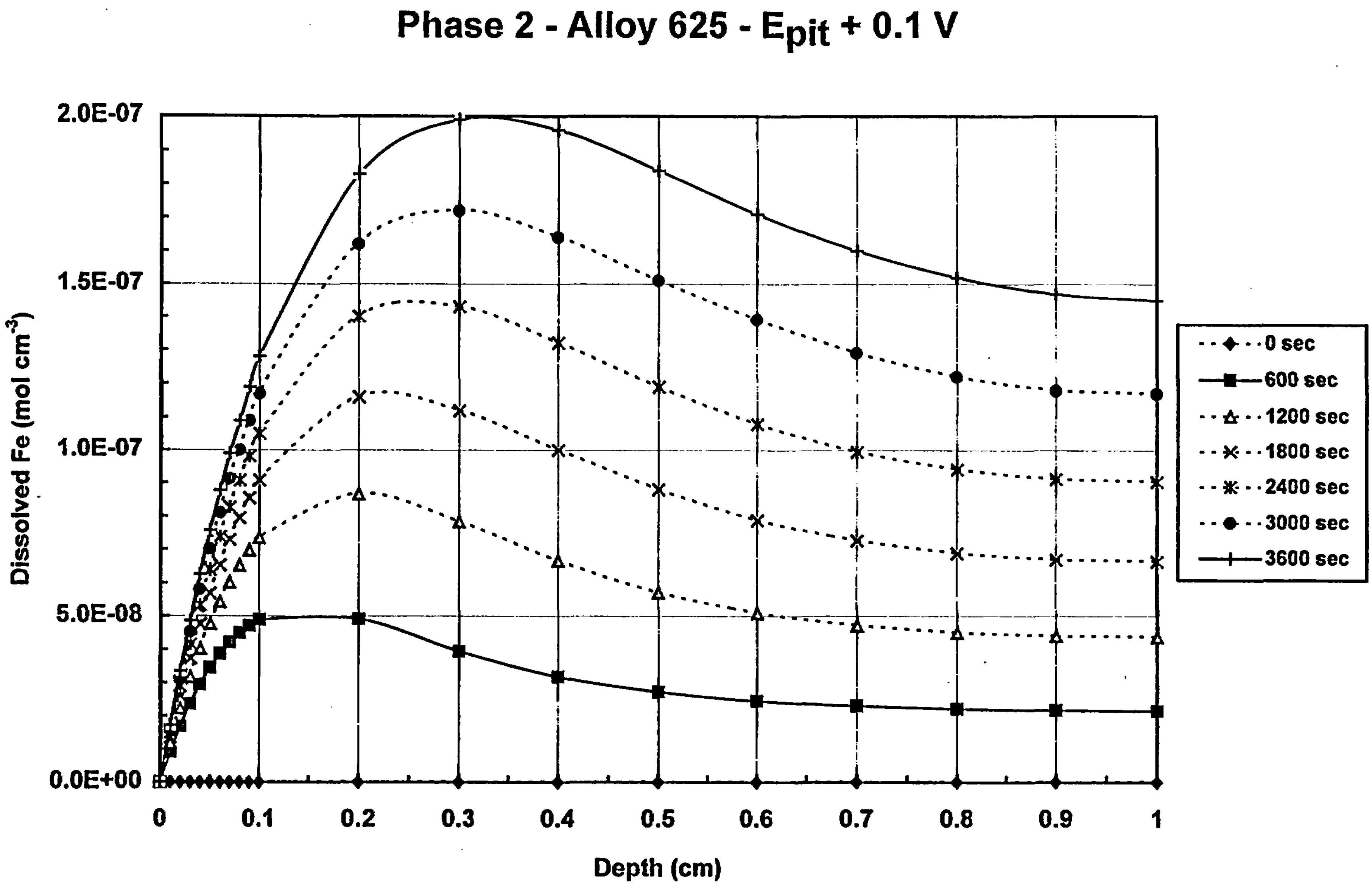

Phase 2 - Alloy 625 - Epit + 0.1 V
Dissolved Fe (mol cm-3)
2.0E-07
1.5E-07
1.0E-07
5.0E-08
0.0E+00
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Fig 8

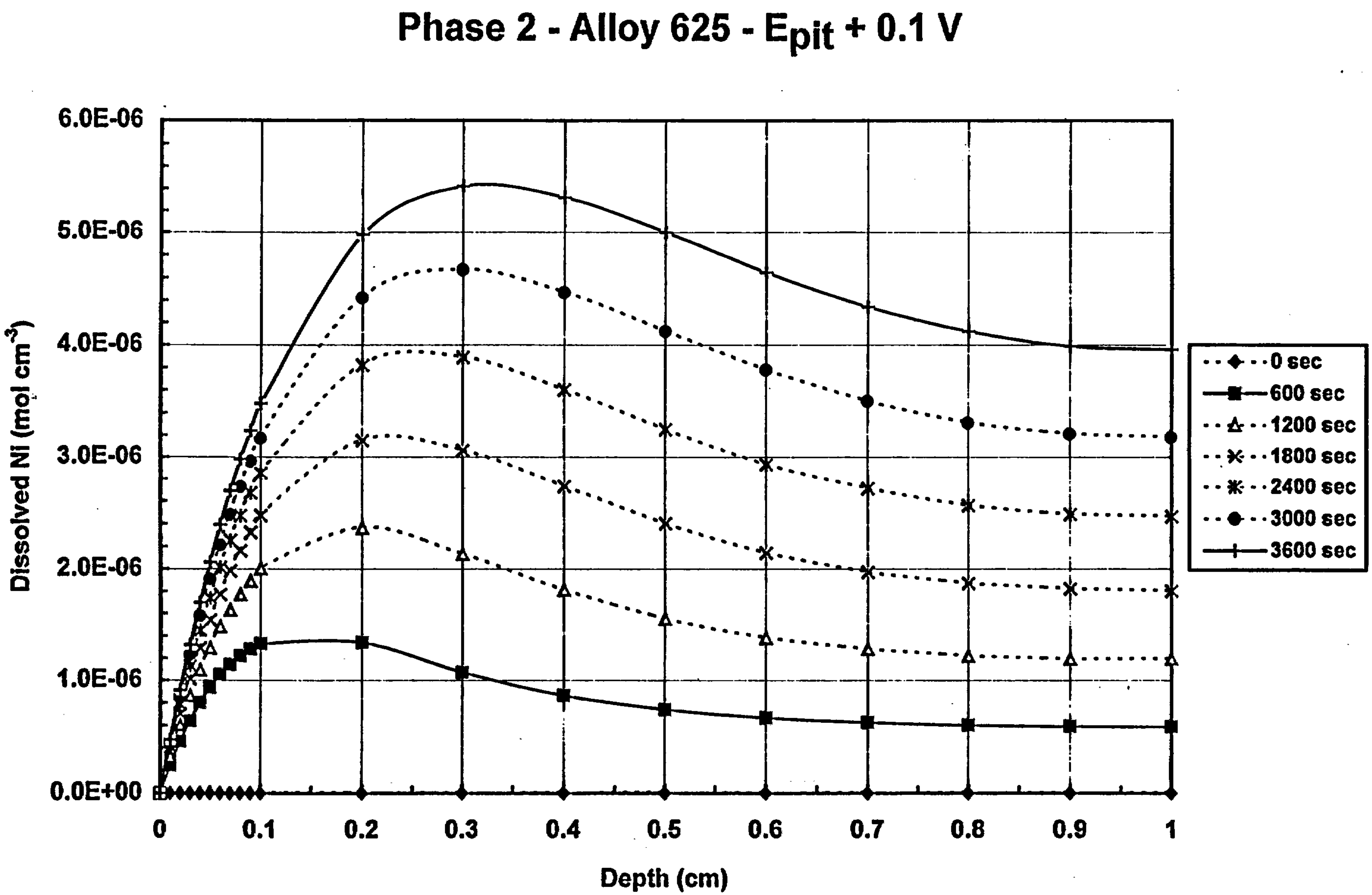

Phase 2 - Alloy 625 - Epit + 0.1 V
Dissolved Ni (mol cm-3)
6.0E-06
5.0E-06
4.0E-06
3.0E-06
2.0E-06
1.0E-06
0.0E+00
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Figure 9

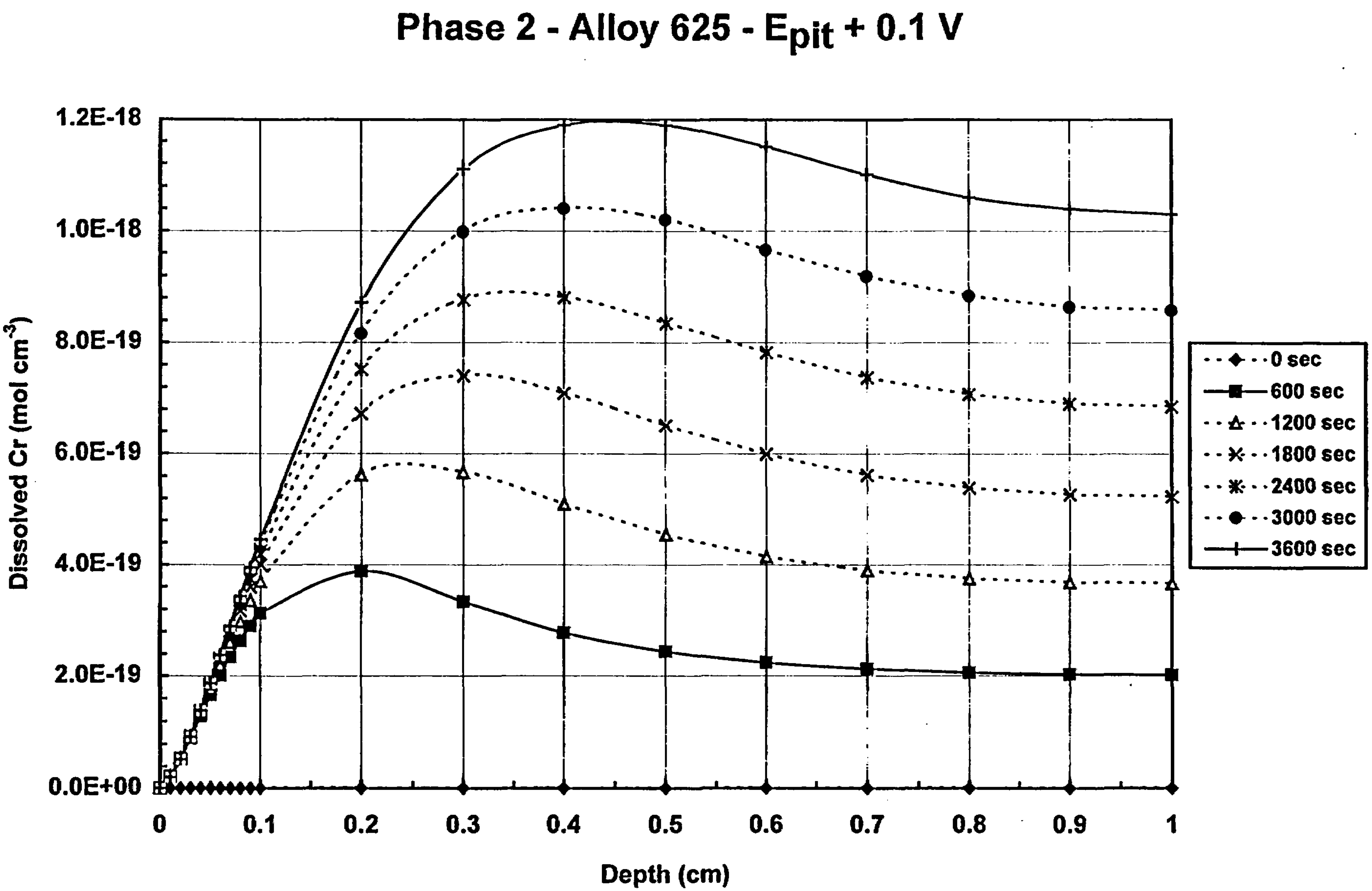

Phase 2 - Alloy 625 - Epit + 0.1 V
1.2E-18
1.0E-18
8.0E-19
6.0E-19
4.0E-19
2.0E-19
0.0E+00
Dissolved Cr (mol cm-3)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Fig 10

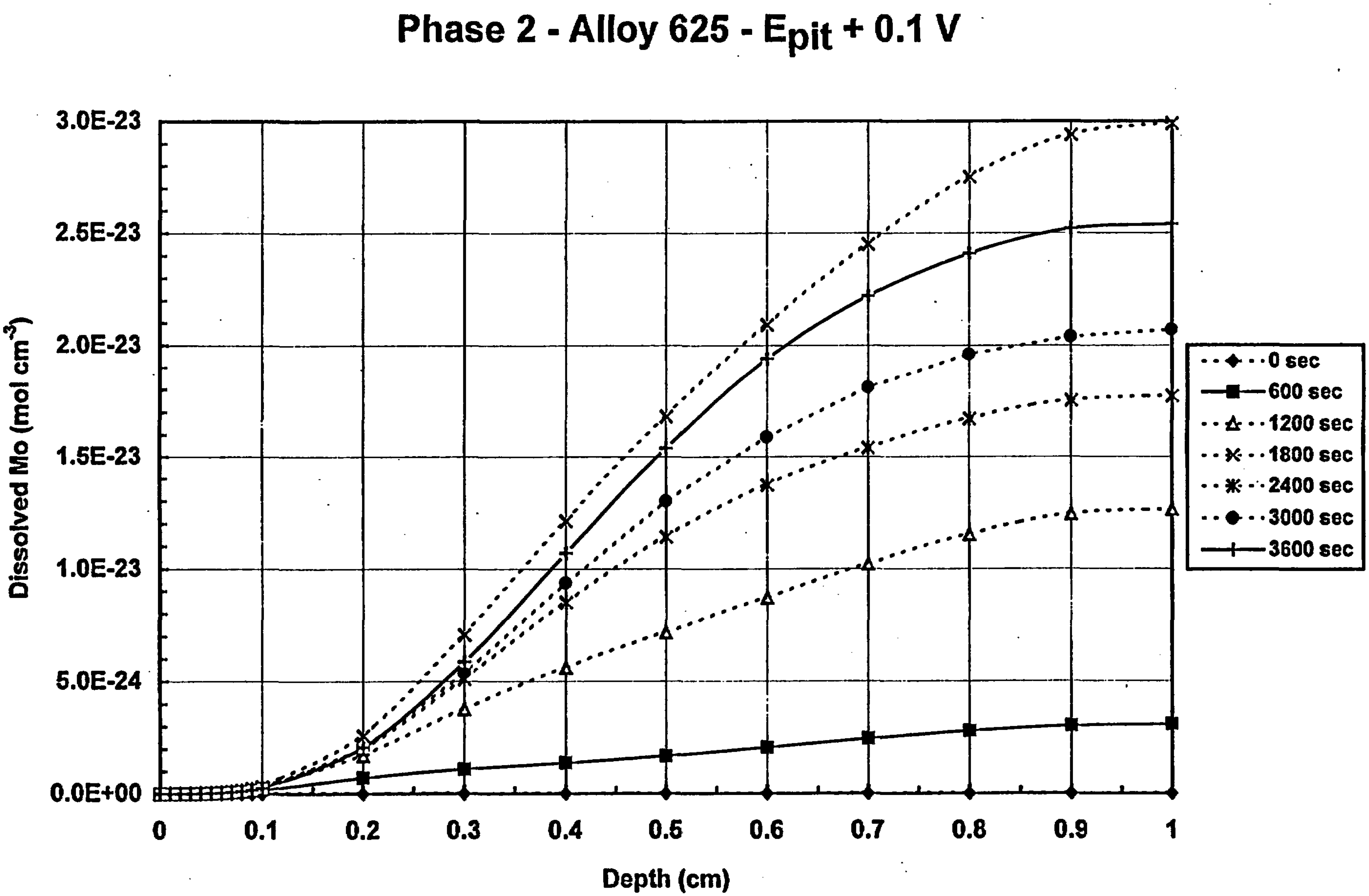

Phase 2 - Alloy 625 - Epit + 0.1 V
3.0E-23
2.5E-23
2.0E-23
1.5E-23
1.0E-23
5.0E-24
0.0E+00
Dissolved Mo (mol cm-3)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Figure 11

Approaches for estimating pH suppression

- **Transport & accumulation of H⁺ - rate expression based upon hydrolysis**

$$\frac{d[H^+]}{dt}=\frac{\left\{\frac{K_{3,1}}{[H^+]}\frac{d[Fe^{2+}]}{dt}+\frac{K_{4,1}}{[H^+]}\frac{d[Fe^{3+}]}{dt}+\frac{K_{5,1}}{[H^+]}\frac{d[Ni^{2+}]}{dt}+\frac{K_{1,1}}{[H^+]}\frac{d[Cr^{3+}]}{dt}+\frac{2K_{1,1}K_{1,2}}{[H^+]^2}\frac{d[Cr^{3+}]}{dt}-2\frac{d[H_2]}{dt}-4\frac{d[O_2]}{dt}\right\}}{\left\{1+\frac{K_{3,1}[Fe^{2+}]}{[H^+]^2}+\frac{K_{4,1}[Fe^{3+}]}{[H^+]^2}+\frac{K_{5,1}[Ni^{2+}]}{[H^+]^2}+\frac{K_{1,1}[Cr^{3+}]}{[H^+]^2}+\frac{4K_{1,1}K_{1,2}[Cr^{3+}]}{[H^+]^3}\right\}}$$

- **Field-driven electromigration of Cl⁻ - electroneutrality**

$$\frac{K_w}{[H^+]}+[Cl^-]+2[SO_4^{2-}]=[H^+]+[Na^+]+2[Fe^{2+}]+3[Fe^{3+}]+2[Ni^{2+}]+3[Cr^{3+}]+$$
$$[Fe(OH)^+]+2[Fe(OH)^{2+}]+[Ni(OH)^+]+2[Cr(OH)^{2+}]+[Cr(OH)_2^+]$$

- **Hydrolysis equilibrium constants can be found in the literature**

Species	i	Ref.	$K_{i,1}$	$K_{i,2}$	$K_{i,3}$	$K_{i,4}$	$K_{i,5}$	$K_{i,5}$
Cr(III)	1	B,C	1.58×10^{-4}	6.31×10^{-7}	4.0×10^{-38}	2.00×10^{3}	3.16×10^{4}	3.16×10^{3}
Cr(VI)	2	C	6.92×10^{-11}					
Fe(II)	3	B	5.0×10^{-9}		7.9×10^{-16}			
Fe(III)	4	A	1.84×10^{-3}	unknown	unknown			
Ni(II)	5	B	3.16×10^{-4}		1.35×10^{-15}			

Approaches for estimating pH suppression (cont'd.)

- **Observed pH suppression**

Salt	1 N	3 N	Saturated	Ref.
$CrCl_3$	1.1	-0.3	-1.4	D
$FeCl_2$	2.1	0.8	0.2	D
$NiCl_2$	3.0	2.7	2.7	D

- **References**

A. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Ed., John Wiley & Sons, New York, NY, 1988, pp. 679-755.

B. J. W. Oldfield, W. H. Sutton, "Crevice Corrosion of Stainless Steels: I. A Mathematical Model," British Corrosion Journal, Vol. 13, No. 1, 1978, pp. 13-22.

C. F. Y. Saleh, G. E. Mbamalu, Q. H. Jaradat, C. E. Brungardt, "Ion Chromatography: Photodiode Array UV-Visible Detection of Cr(III) Hydrolytic Polymerization Products in Pure and Natural Waters, Analytical Chemistry, Vol. 68, No. 5, March 1, 1996, pp. 740-745.

D. D. A. Jones, B. E. Wilde, "Galvanic Reactions During Localized Corrosion on Stainless Steel, Corrosion Science, Vol. 18, 1978, pp. 631-643.

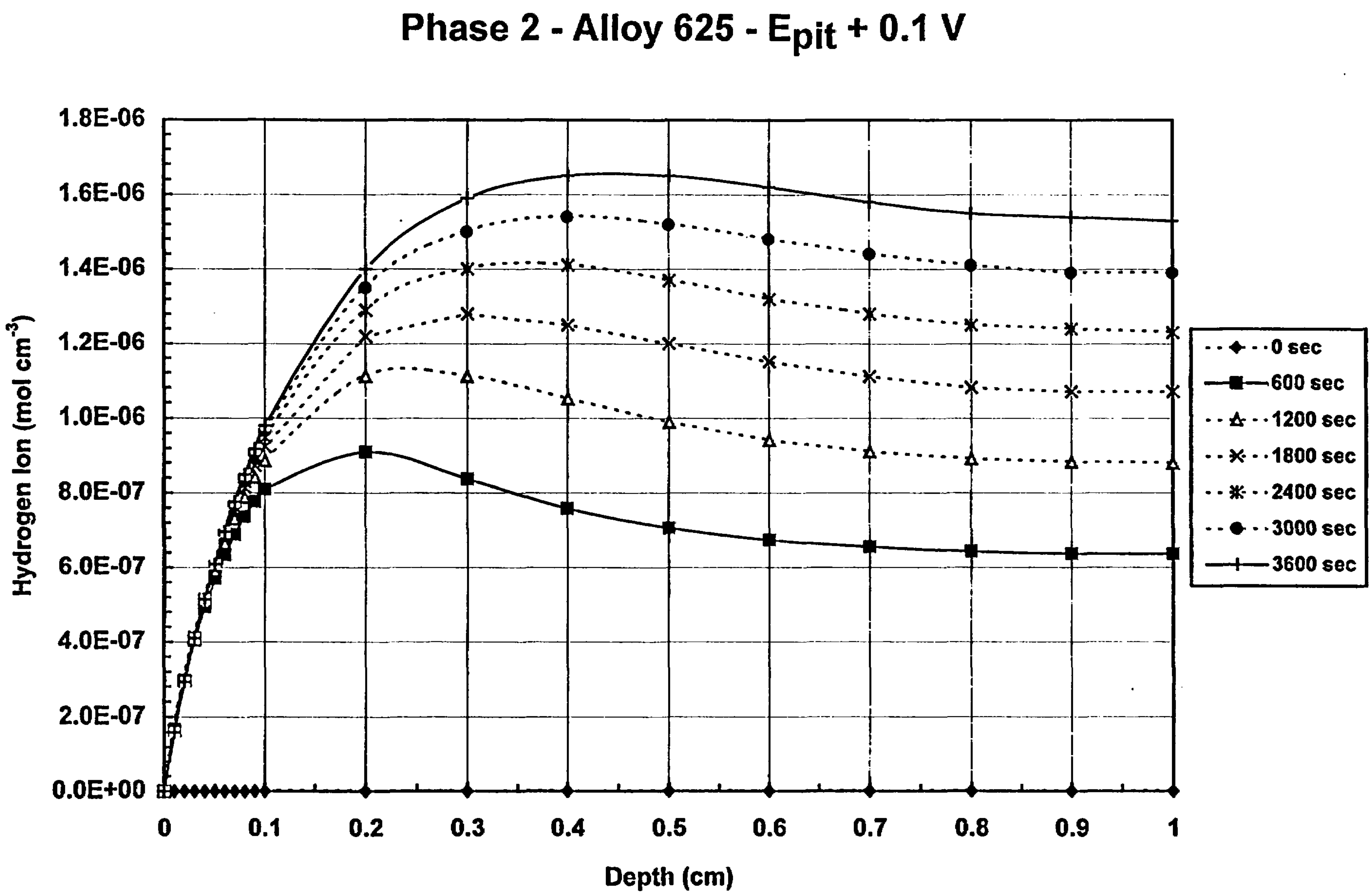

Phase 2 - Alloy 625 - Epit + 0.1 V
1.8E-06
1.6E-06
1.4E-06
1.2E-06
1.0E-06
8.0E-07
6.0E-07
4.0E-07
2.0E-07
0.0E+00
Hydrogen Ion (mol cm-3)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Figure 12

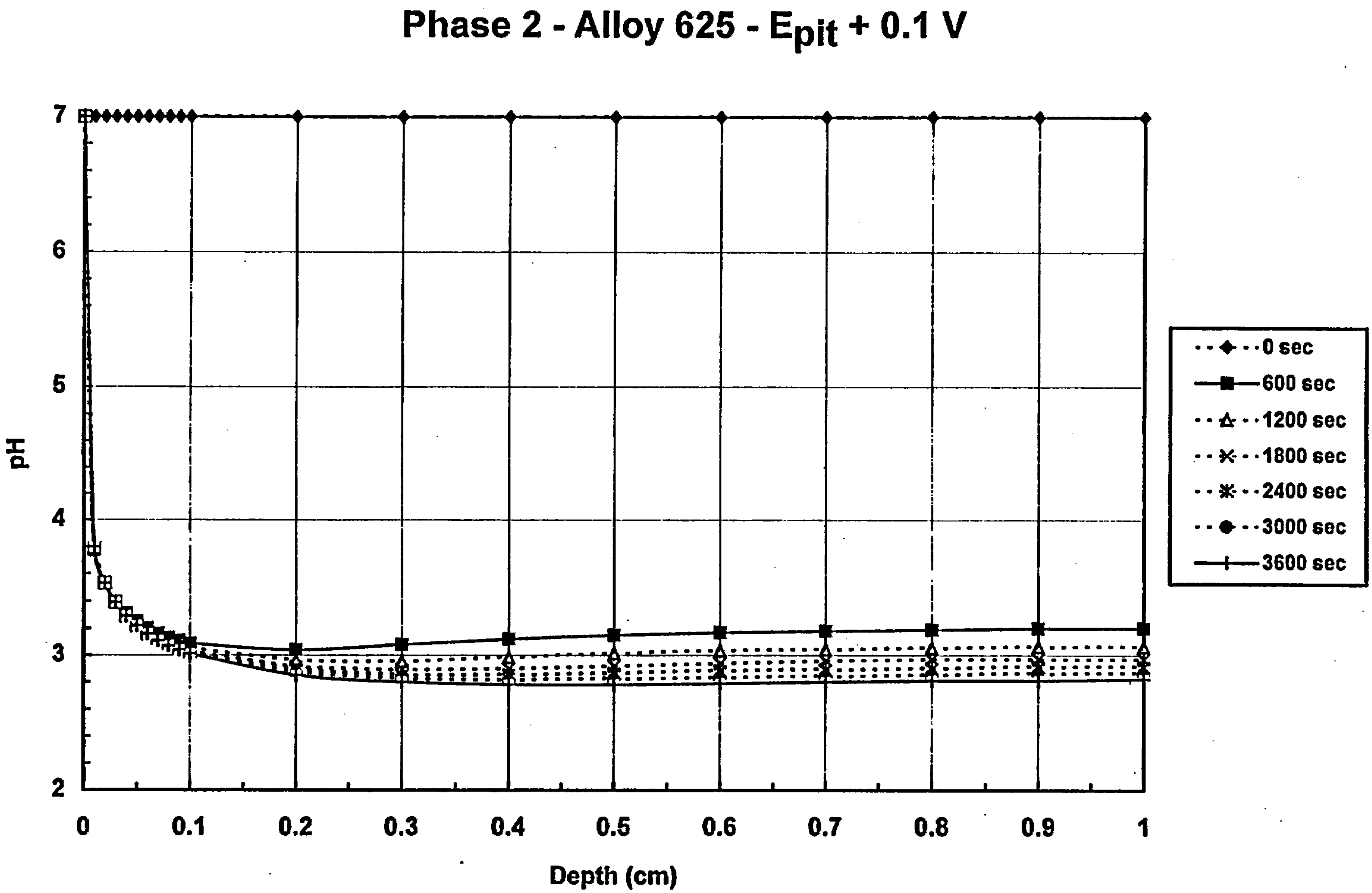

Phase 2 - Alloy 625 - Epit + 0.1 V
pH
7
6
5
4
3
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Figure 13

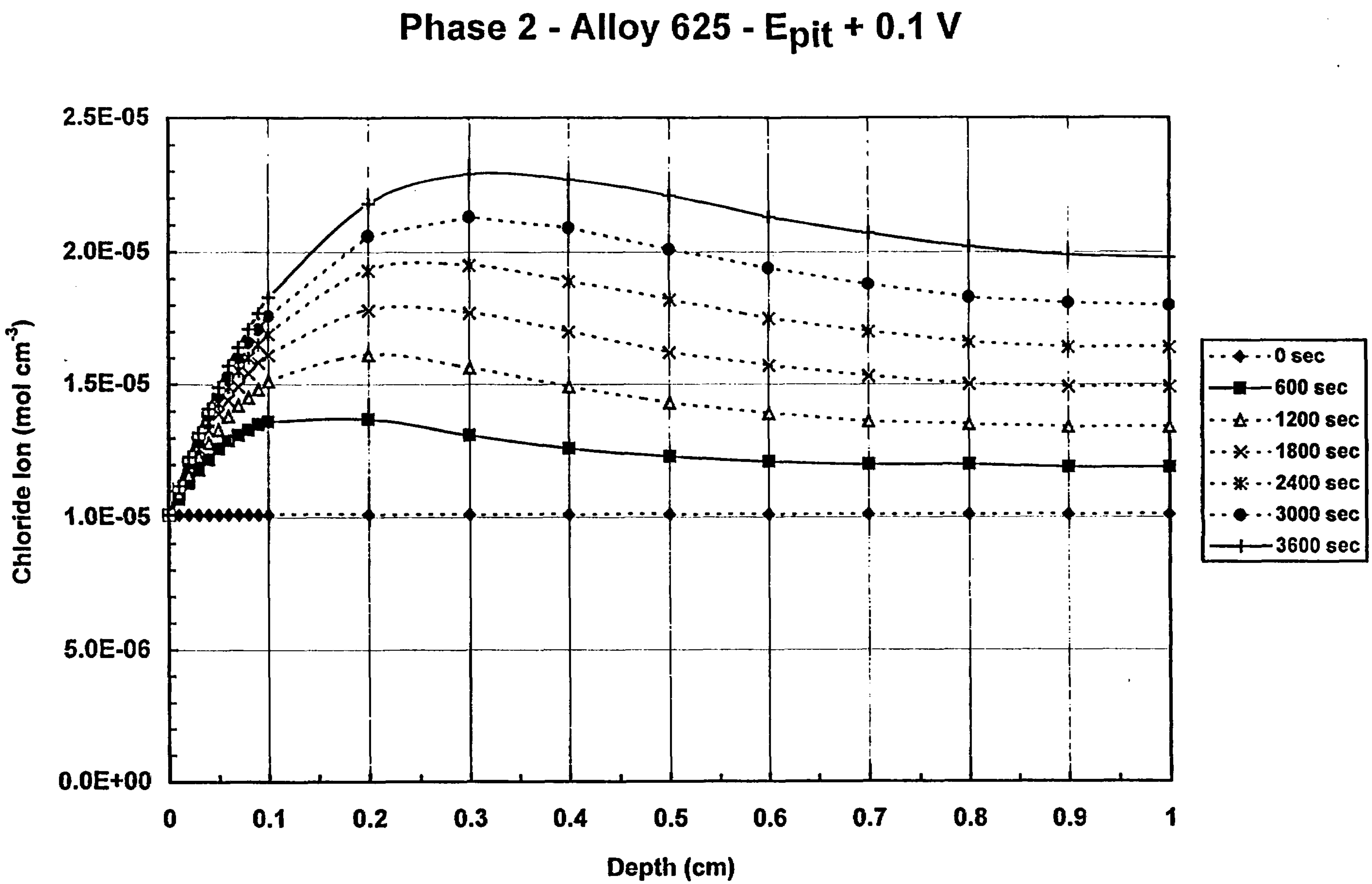

Phase 2 - Alloy 625 - E_{pit} + 0.1 V
2.5E-05
2.0E-05
1.5E-05
1.0E-05
5.0E-06
0.0E+00
Chloride Ion (mol cm^{-3})
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Fig 14

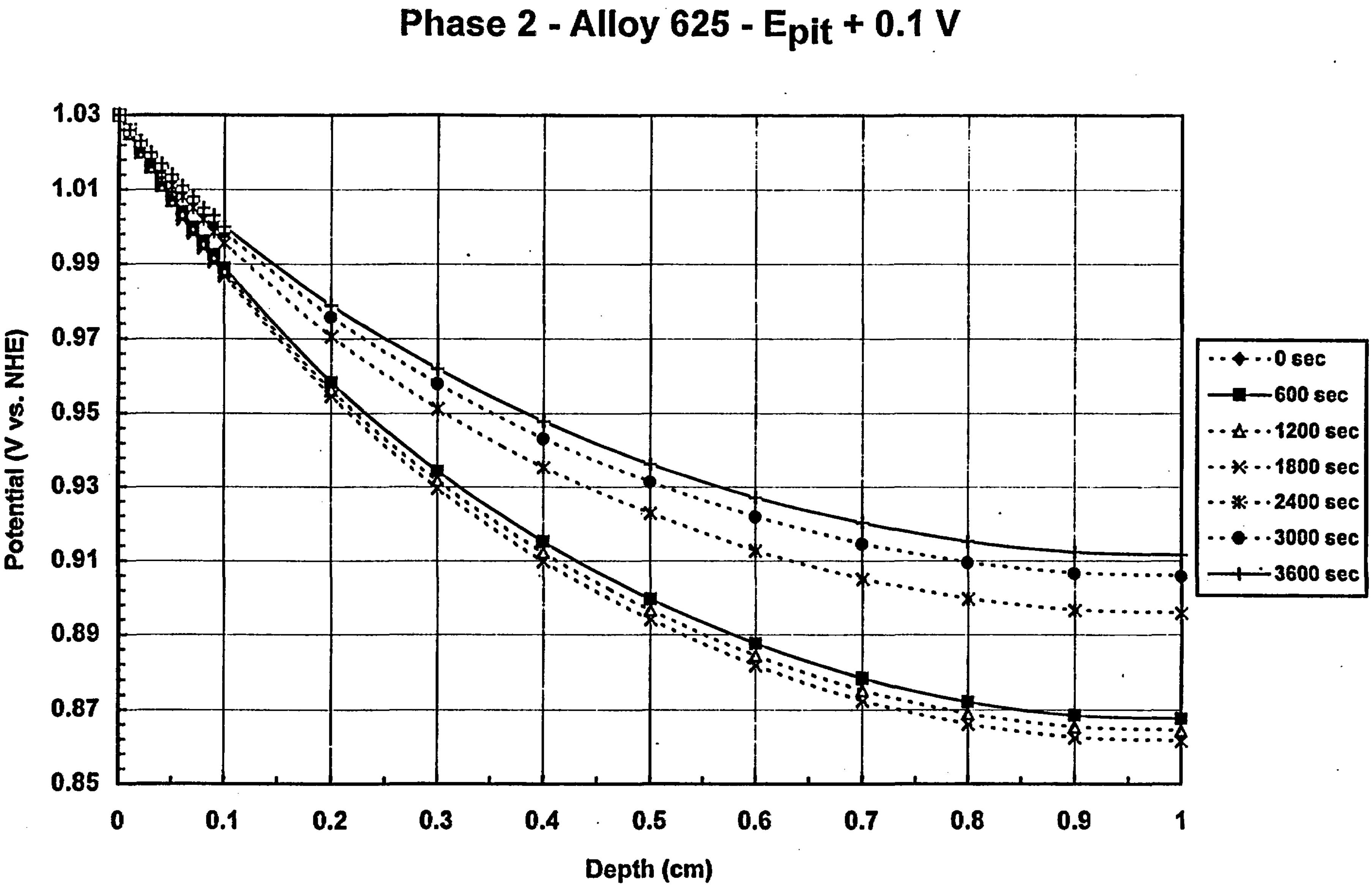

Phase 2 - Alloy 625 - Epit + 0.1 V
Potential (V vs. NHE)
1.03
1.01
0.99
0.97
0.95
0.93
0.91
0.89
0.87
0.85
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Figure 15

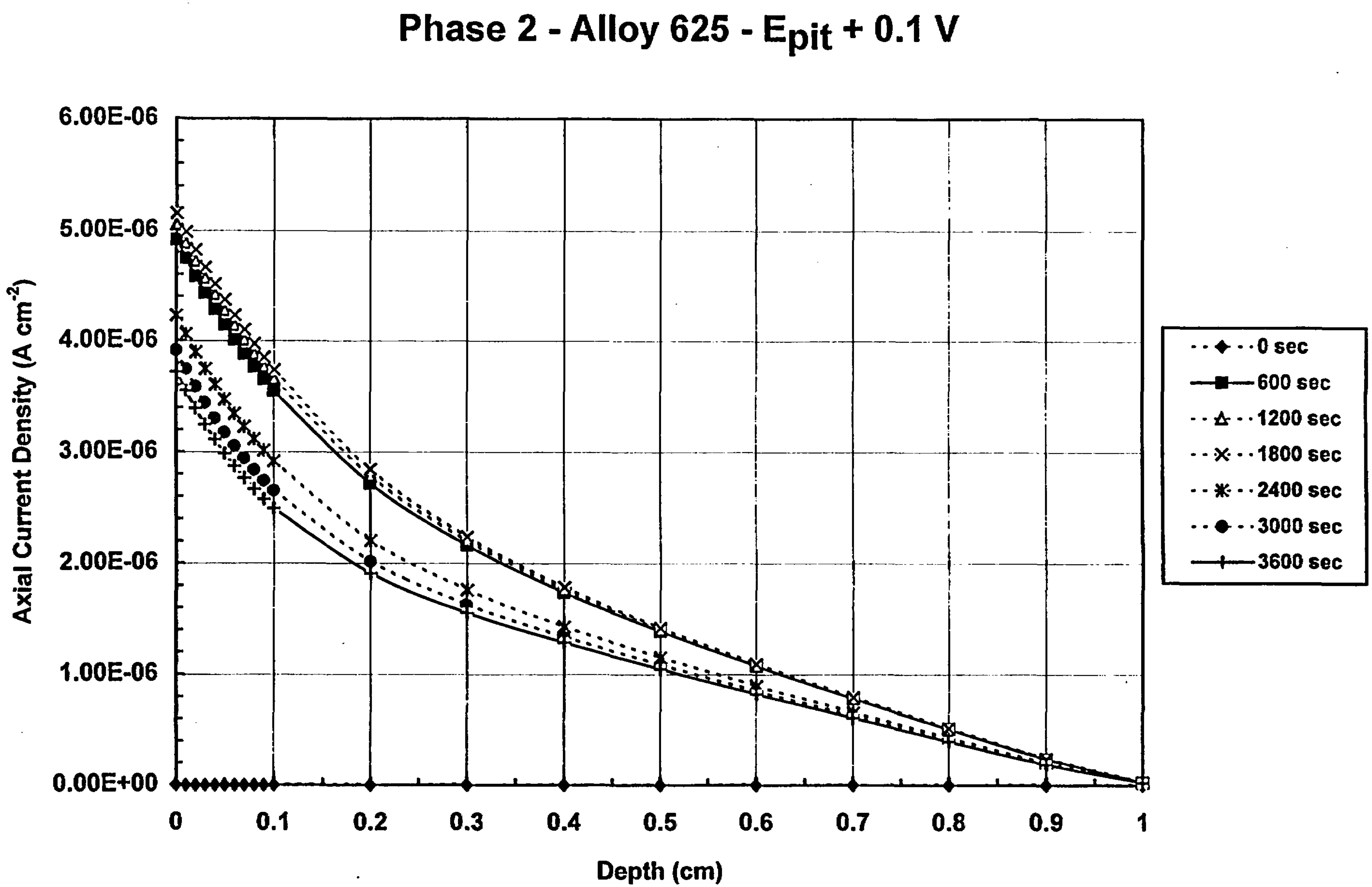
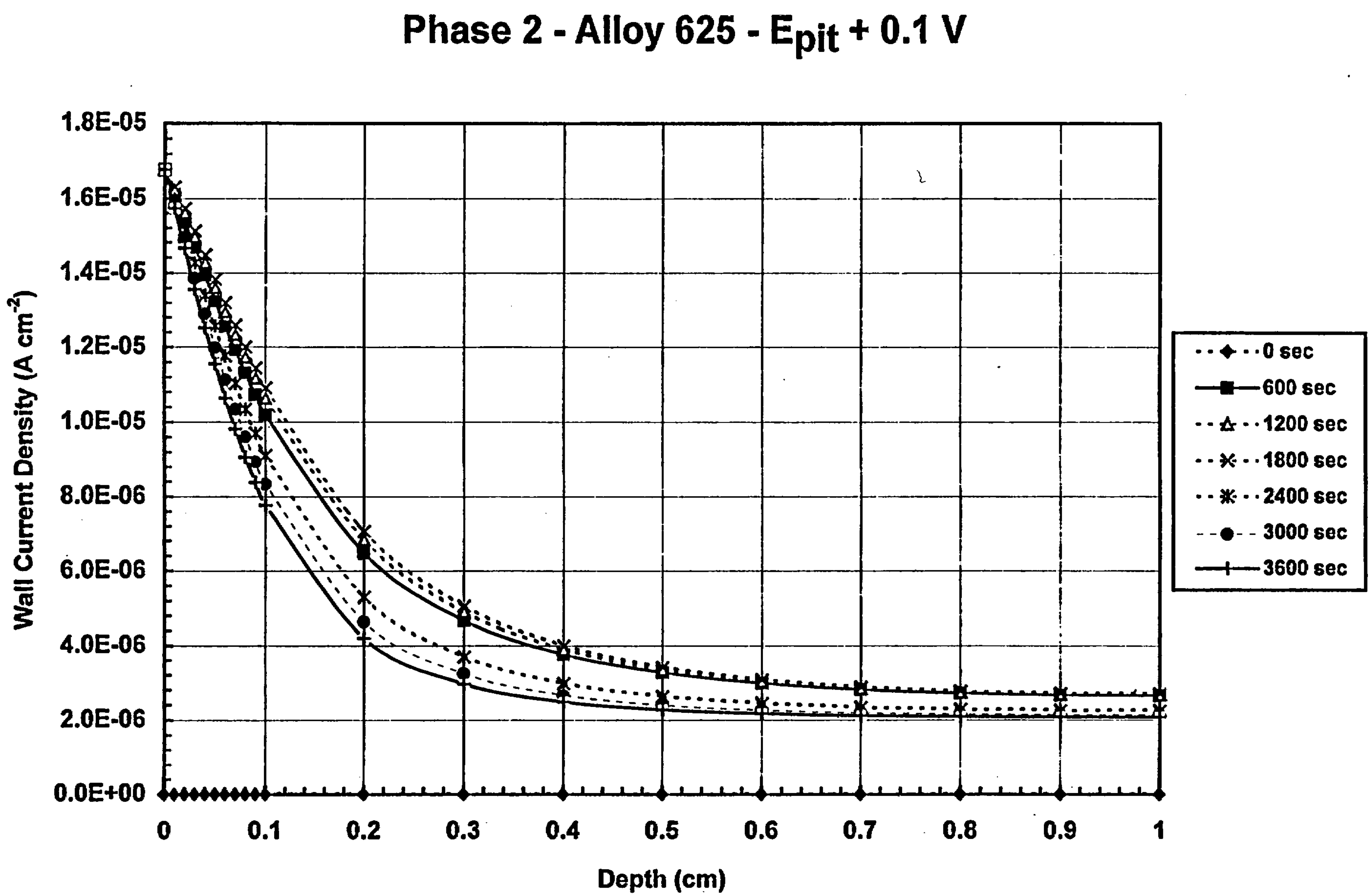

Phase 2 - Alloy 625 - E_{pit} + 0.1 V
6.00E-06
5.00E-06
4.00E-06
3.00E-06
2.00E-06
1.00E-06
0.00E+00
Axial Current Density (A cm^{-2})
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Figure 16



Phase 2 - Alloy 625 - E_{pit} + 0.1 V
1.8E-05
1.6E-05
1.4E-05
1.2E-05
1.0E-05
8.0E-06
6.0E-06
4.0E-06
2.0E-06
0.0E+00
Wall Current Density (A cm^{-2})
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Depth (cm)
0 sec
600 sec
1200 sec
1800 sec
2400 sec
3000 sec
3600 sec

Figure 17

Pitting models

- Pit initiation
  - Halide nuclei theory (Okada)
  - Point defect model (Chao, Lin & McDonald)
  - Electrostriction model (Sato)
  - Stochastic probability theory (Shibata; Henshall; Farmer)

- Pit propagation
  - Pickering-Frankenthal model
    - Estimates potential drop & concentration gradients
    - Assumes passive walls & active base
    - Does not account for hydrolysis reactions
  - Galvele modification of Pickering-Frankenthal model
    - Accounts for single hydrolysis reaction & pH suppression
  - Beck-Alkire model
    - Assumes semispherical pit
    - Thin electrically-resistive halide film

Early probabilistic pitting model developed for YMP

- Container surface is divided into hypothetical "cells" where probabilities for the transition from one pitting state to another can be assigned
- Nucleation or death of a pit "embryo" is determined by comparing random numbers (generated by power residue method) to:
  - Birth probability (λ)
  - Death probability (μ)
- An "embryo" becomes a "stable pit" after a critical age (τ) is reached
  - The depth of a "stable pit" is calculated from its age
- Several deficiencies in this early model are evident
  - Birth & death probabilities depend upon E, Cl^-, and T
  - The effects of pH and alloy composition are not included
  - Calculated probabilities can be >> 1 (code limits values to ~ 1)
  - The birth probability is assumed to decay time

Probabilistic pitting model in present form

- **Embryo birth**

$$\lambda_1 = \lambda_0 \left[Cl^-\right] \exp\left(\frac{\alpha_\lambda F}{RT}\left(E - E_{crit}\right)\right) \qquad \lambda = 1 - e^{-\lambda_1 \delta t} \qquad \lambda = \lambda\left(A\, \theta_P{}^n \exp\left[-B\, \theta_P\right]\right)$$

- **Embryo death**

$$\mu_1 = \mu_0 \left[OH^-\right] \exp\left(-\frac{\alpha_\mu F}{RT}\left(E - E_{pass}\right)\right) \qquad \mu = 1 - e^{-\mu_1 \delta t}$$

- **Stable pit generation**

$$\gamma_1 = \gamma_0 \exp\left(-\frac{A_\gamma}{RT}\right) \qquad \gamma = 1 - e^{-\gamma_1 \delta t}$$

- **Incubation time concept**

$$\tau_1 = \tau_0 \exp\left(-\frac{A_\tau}{RT}\right)$$

- **Pit Growth & Stifling**

$$d = \sqrt{2\, K\, \mathrm{T}_{age}} \qquad \frac{i_{pass}}{4F} \leq D \left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0}$$

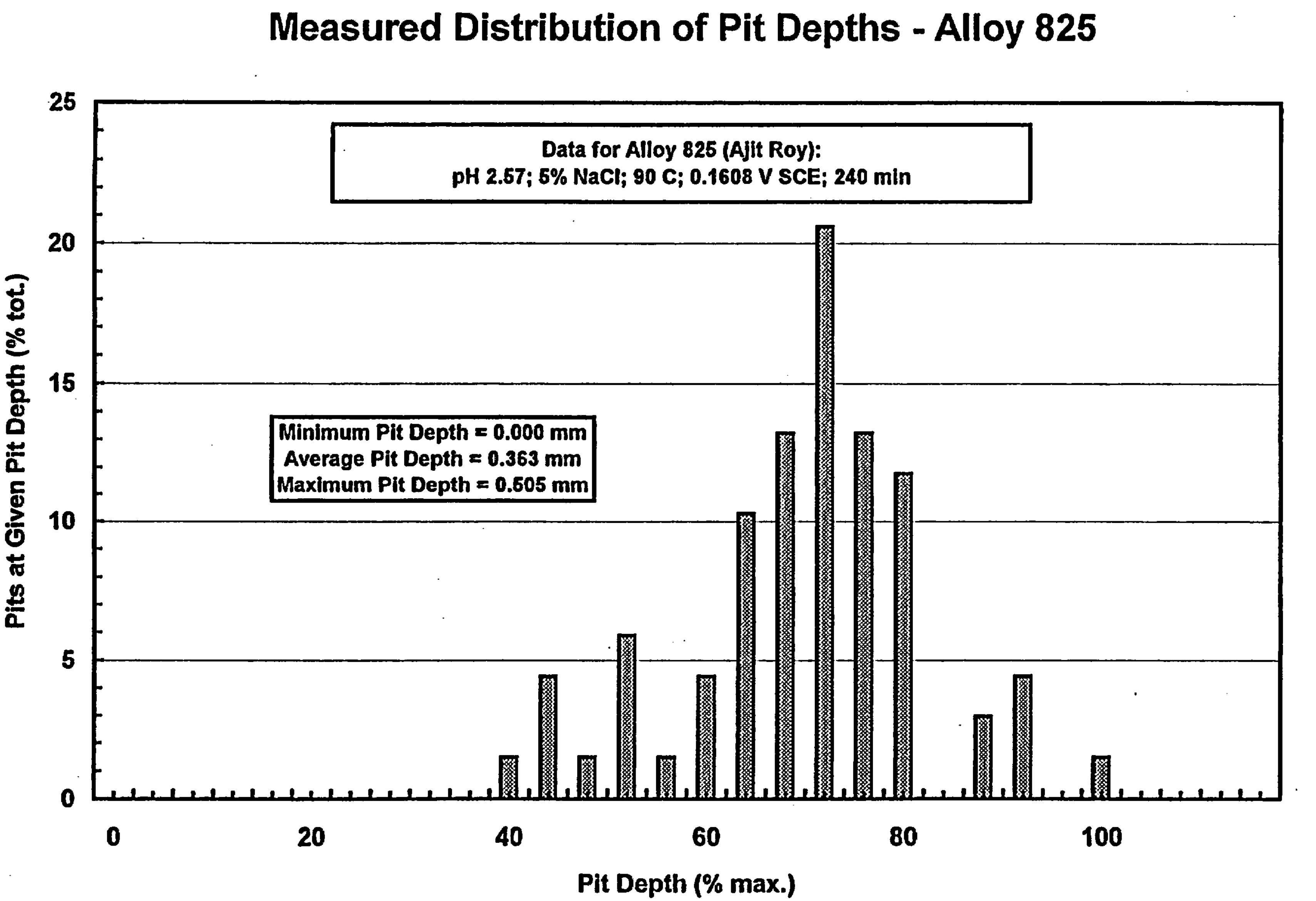

Measured Distribution of Pit Depths - Alloy 825
Data for Alloy 825 (Ajit Roy):
pH 2.57; 5% NaCl; 90 C; 0.1608 V SCE; 240 min
Minimum Pit Depth = 0.000 mm
Average Pit Depth = 0.363 mm
Maximum Pit Depth = 0.505 mm
Pits at Given Pit Depth (% tot.)
Pit Depth (% max.)
0
5
10
15
20
25
0
20
40
60
80
100

Figure 18

Predicted Transients in Surface Coverage - Alloy 825

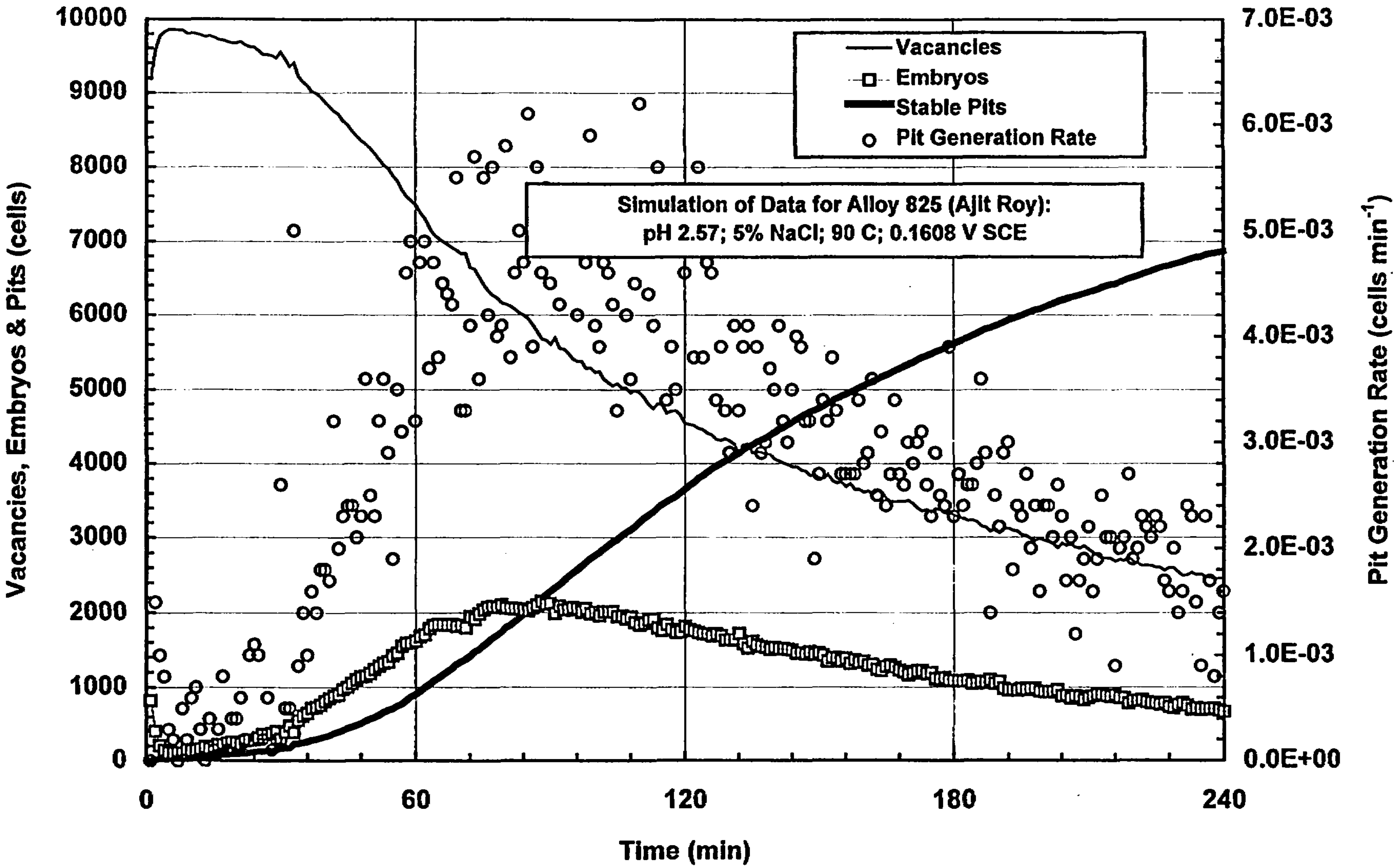


Figure 19

Predicted Distribution of Pit Depths - Alloy 825

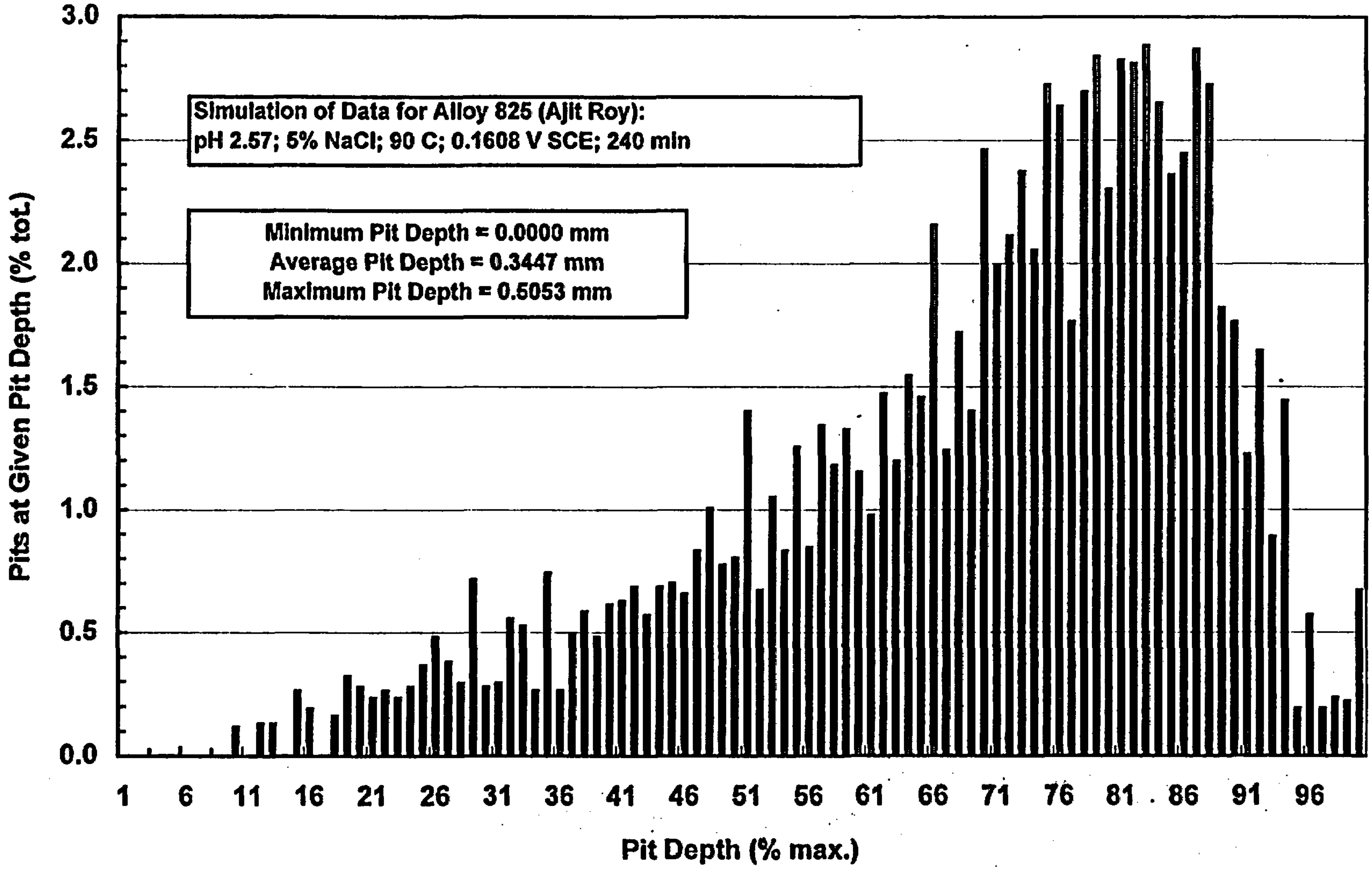


Figure 20

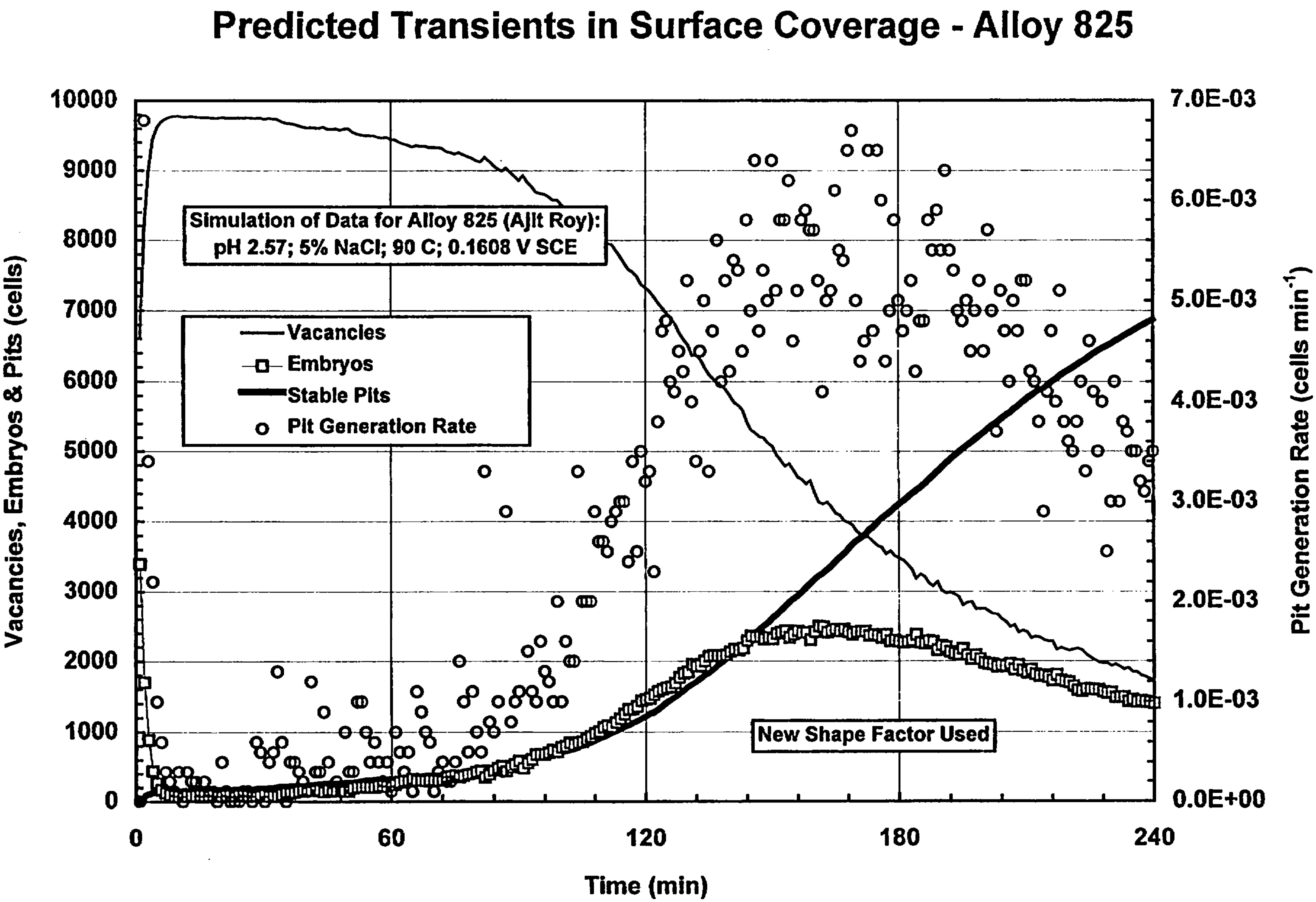

Predicted Transients in Surface Coverage - Alloy 825
Simulation of Data for Alloy 825 (Ajit Roy):
pH 2.57; 5% NaCl; 90 C; 0.1608 V SCE
Vacancies
Embryos
Stable Pits
Pit Generation Rate
New Shape Factor Used
Vacancies, Embryos & Pits (cells)
Pit Generation Rate (cells min^{-1})
Time (min)
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
7.0E-03
6.0E-03
5.0E-03
4.0E-03
3.0E-03
2.0E-03
1.0E-03
0.0E+00
0
60
120
180
240

Figure 21

Predicted Distribution of Pit Depths - Alloy 825

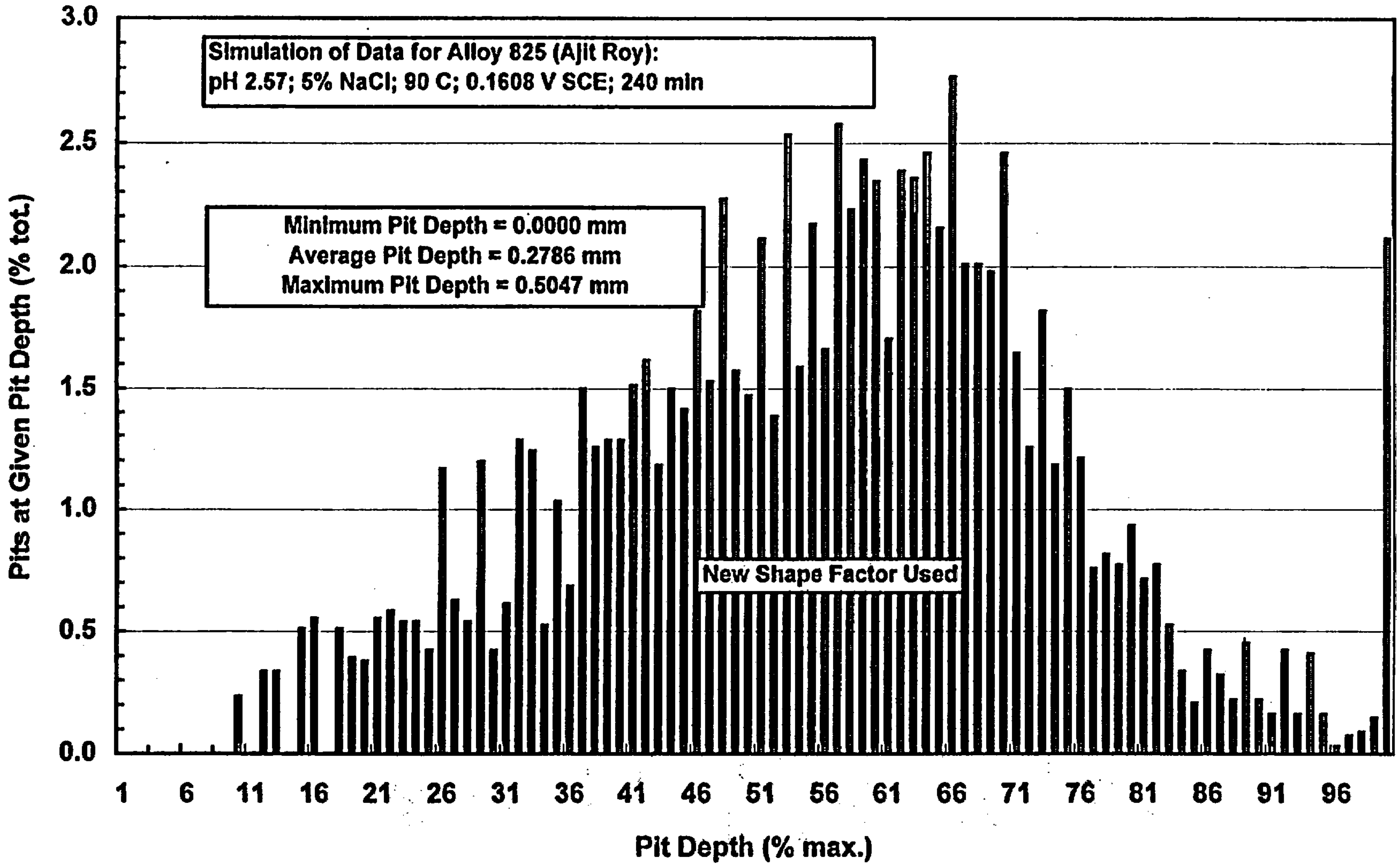


Figure 22

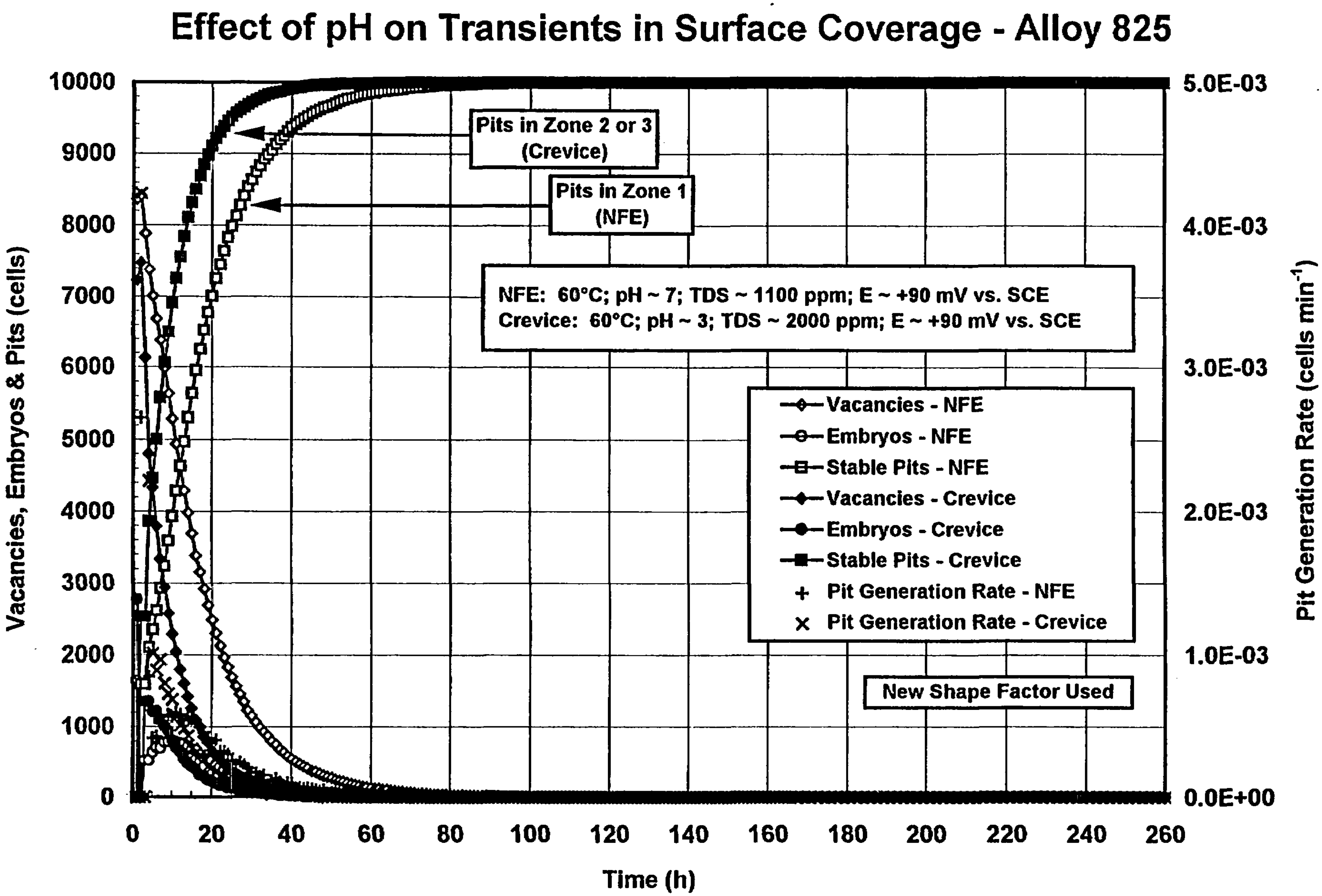
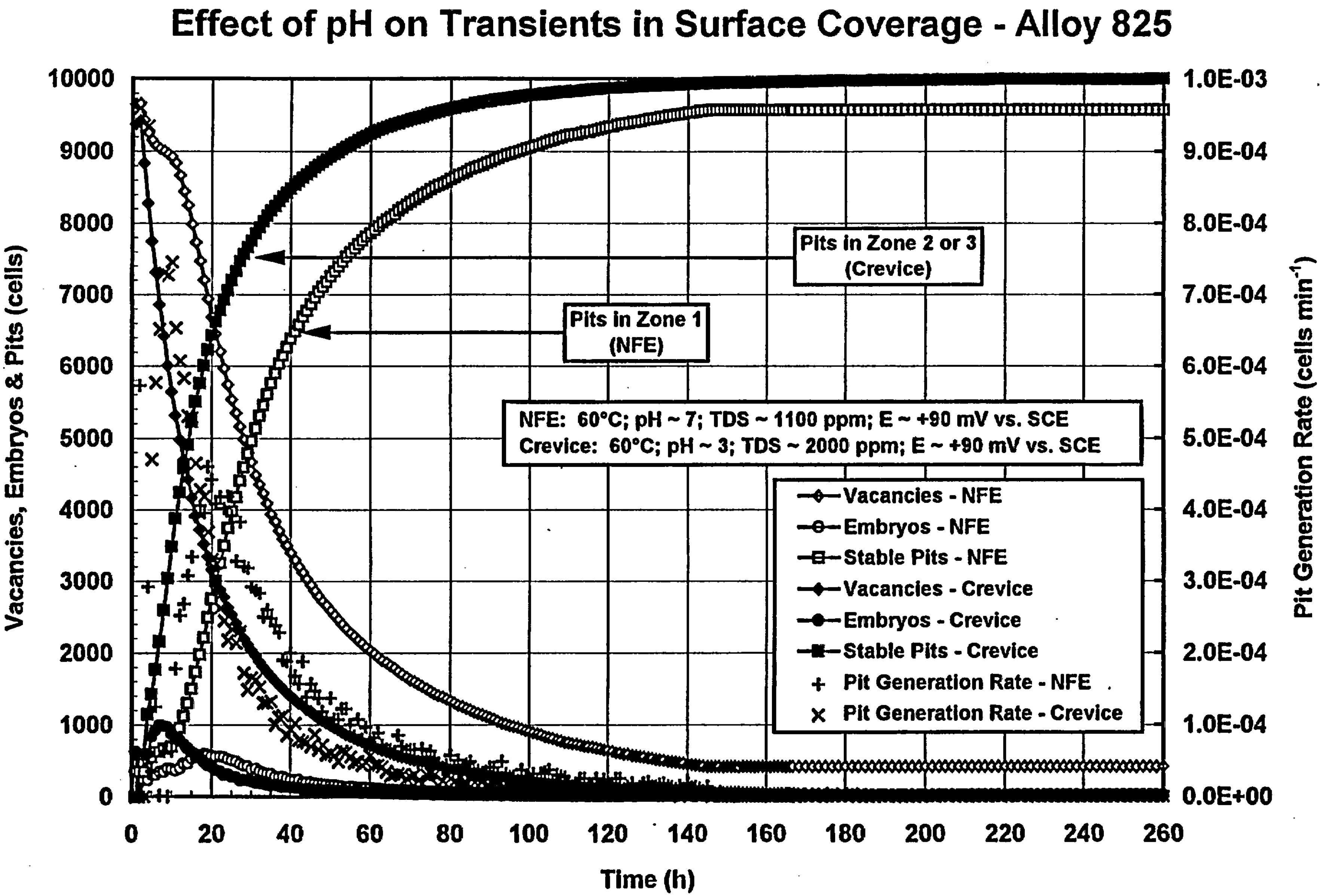
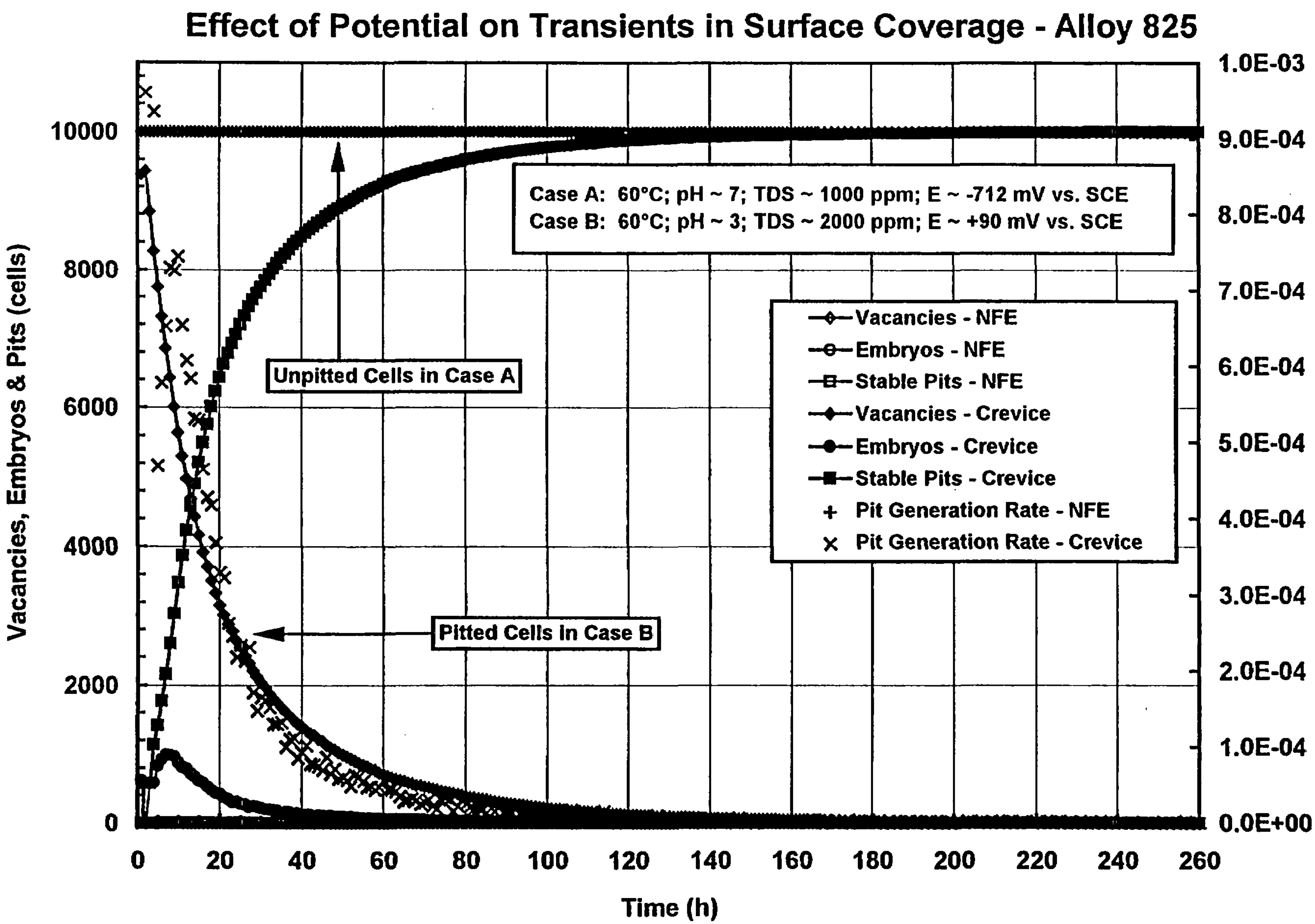

Effect of pH on Transients in Surface Coverage - Alloy 825
Vacancies, Embryos & Pits (cells)
Pit Generation Rate (cells min^{-1})
Time (h)
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
5.0E-03
4.0E-03
3.0E-03
2.0E-03
1.0E-03
0.0E+00
0
20
40
60
80
100
120
140
160
180
200
220
240
260
Pits in Zone 2 or 3 (Crevice)
Pits in Zone 1 (NFE)
NFE: 60°C; pH ~ 7; TDS ~ 1100 ppm; E ~ +90 mV vs. SCE
Crevice: 60°C; pH ~ 3; TDS ~ 2000 ppm; E ~ +90 mV vs. SCE
Vacancies - NFE
Embryos - NFE
Stable Pits - NFE
Vacancies - Crevice
Embryos - Crevice
Stable Pits - Crevice
Pit Generation Rate - NFE
Pit Generation Rate - Crevice
New Shape Factor Used

Figure 25



Effect of pH on Transients in Surface Coverage - Alloy 825
Vacancies, Embryos & Pits (cells)
Pit Generation Rate (cells min⁻¹)
Time (h)
0
20
40
60
80
100
120
140
160
180
200
220
240
260
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
0.0E+00
1.0E-04
2.0E-04
3.0E-04
4.0E-04
5.0E-04
6.0E-04
7.0E-04
8.0E-04
9.0E-04
1.0E-03
Pits in Zone 2 or 3 (Crevice)
Pits in Zone 1 (NFE)
NFE: 60°C; pH ~ 7; TDS ~ 1100 ppm; E ~ +90 mV vs. SCE
Crevice: 60°C; pH ~ 3; TDS ~ 2000 ppm; E ~ +90 mV vs. SCE
Vacancies - NFE
Embryos - NFE
Stable Pits - NFE
Vacancies - Crevice
Embryos - Crevice
Stable Pits - Crevice
Pit Generation Rate - NFE
Pit Generation Rate - Crevice

Figure 23



Effect of Potential on Transients in Surface Coverage - Alloy 825
Case A: 60°C; pH ~ 7; TDS ~ 1000 ppm; E ~ -712 mV vs. SCE
Case B: 60°C; pH ~ 3; TDS ~ 2000 ppm; E ~ +90 mV vs. SCE
Unpitted Cells in Case A
Pitted Cells in Case B
Vacancies - NFE
Embryos - NFE
Stable Pits - NFE
Vacancies - Crevice
Embryos - Crevice
Stable Pits - Crevice
Pit Generation Rate - NFE
Pit Generation Rate - Crevice
Vacancies, Embryos & Pits (cells)
Pit Generation Rate (cells min⁻¹)
Time (h)
0
2000
4000
6000
8000
10000
0.0E+00
1.0E-04
2.0E-04
3.0E-04
4.0E-04
5.0E-04
6.0E-04
7.0E-04
8.0E-04
9.0E-04
1.0E-03
0 20 40 60 80 100 120 140 160 180 200 220 240 260

Fig' ⁀'7

Equivalent deterministic & probabilistic models

- Transition between two states - birth & death of an embryo (Shibata)

$$P_0 + P_1 = 1$$

$$\frac{dP_0}{dt} = -\lambda_0 P_0 + \mu_1(1 - P_0)$$

- Kinetics associated with adsorption isotherm (Langmuir)

$$\theta_{ads} + \theta_{vac} = 1$$

$$\frac{d\theta_{ads}}{dt} = -k_b \theta_{ads} + k_f C(1 - \theta_{ads})$$

- The deterministic approach offers computational advantages

Equivalent deterministic pitting model - details

- **More complete statement of problem**

$$\theta_E + \theta_V + \theta_P = 1$$

$$\frac{d\theta_E}{dt} = k_{birth}\left[Cl^-\right]^a (1-\theta_E-\theta_P) - k_{death}\left[OH^-\right]^b \theta_E - k_{pit}\theta_E$$

$$\frac{d\theta_P}{dt} = k_{pit}\theta_E$$

- **Quasi steady state between facile birth & death processes**

$$k_{pit}\theta_E << k_{birth}\left[Cl^-\right]^a (1-\theta_E) \qquad k_{pit}\theta_E << k_{death}\left[OH^-\right]^b \theta_E$$

$$\theta_E = (1-\theta_P)\left[\frac{G}{1+G}\right] \qquad \theta_P = 1 - \exp\left[-k_{pit}t\frac{G}{1+G}\right] \qquad d \approx A\sqrt{t}$$

$$G = \frac{k_{birth}\left[Cl^-\right]^a\left[H^+\right]^b}{k_{death}K_w^b} \qquad \frac{k_{birth}}{k_{death}} = \frac{k_{birth}^o}{k_{birth}^o} e^{\frac{nF(E-E_c)}{RT}}$$

Summary

- Crevice corrosion
  - A detailed model has been developed
    - Potential & current distributions (limited by E_{mix} in crevice)
    - Transient concentration profiles of reactive species
    - Suppressed pH due to hydrolysis of Fe, Ni, Cr & Mo
  - Several useful conclusions can be drawn from this model
    - The pH will be fairly uniform inside the crevice (pH ~ 2-3)
    - The potential (E) will decrease with increasing depth
    - Chloride (Cl^-) concentration will increase
- Pitting corrosion
  - Expressions for (λ μ γ τ) are now functions of E, T, pH, and Cl^-
    - No pitting of Alloy 825 predicted at E_{corr} of carbon steel
  - Reliable quantitative predictions require additional measurements
    - Pit distributions for Alloys 625 and C-22 (Ajit Roy, LLNL)
    - Birth & death rates of metastable pits (John Scully, U.Va.)

Stress corrosion cracking models

- Stress corrosion crack initiation
  - Model based on displacement at crack tip (Buck & Ranjan)
  - Model for initiation of crack at elliptical pit (Hagn)
  - Model for sensitization due to $M_{23}C_6$ precipitation at grain boundaries (Bain; Stawstrom & Hillert; Tedmon)
- Stress corrosion crack propagation
  - Anodic dissolution at crack tip (Turnbull & Thomas)
    - ⇒ Limited by convection, diffusion & electromigration
    - ⇒ Does not account for effects of stress & strain at crack tip
  - Slip-dissolution-repassivation (SDR) model (Nakayama & Takano)
    - ⇒ Periodic film-fracture & repassivation events
  - Film-fracture model (Andresen & Ford; Huang)
    - ⇒ Periodic film-fracture & repassivation events
    - ⇒ Allows for mass transport limitations at crack tip

ATTACHMENT 16

YUCCA MOUNTAIN PROJECT

Studies

Approach to Waste Package Degradation Modeling and Abstraction for TSPA-VA

Presented to:
DOE/NRC Technical Exchange on
Total System Performance Assessment
Las Vegas, NV

Presented by:
Joon H. Lee
Senior Performance Assessment Analyst
CRWMS M&O/Duke Engineering & Services

November 6, 1997

U.S. Department of Energy
Office of Civilian Radioactive
Waste Management

Outline of Presentation

- Introduction
- Conceptual model for waste package degradation Modeling for TSPA-VA
- Base case waste package degradation model for TSPA-VA
- Key parameters for waste package degradation model derived from Waste Package Degradation Expert Elicitation (WPDEE)
- Representation of variability and uncertainty in waste package degradation
- Concluding remarks

Aspects of Waste Package Performance That Impact Total System Performance

- Waste containment - time of waste package failure
  - waste package failure defined as the first perforation (pit penetration or crack propagation) through the container wall
  - corresponds to the initiation of waste form degradation inside the failed waste package

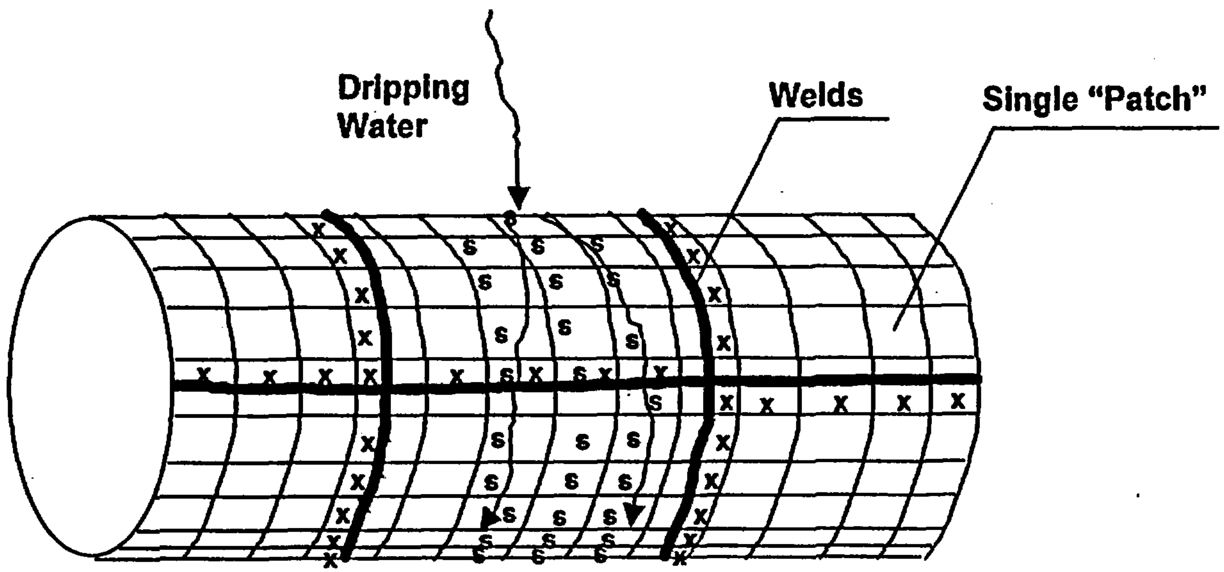
Aspects of Waste Package Performance That Impact Total System Performance
(Continued)

- Controlled/gradual release of radionuclides - waste package failure rate, and subsequent perforation rate of failed waste container
  - waste package failure rate provides the rate of waste inventories that become available for release
  - subsequent perforation rate of failed waste container provides the area in the waste container available for radionuclide transport by diffusion and/or advection

Schematic of the Conceptual Model for WP Degradation Modeling and Abstraction for TSPA-VA

* T, RH, in-drift water dripping across repository from drift-scale T-H model

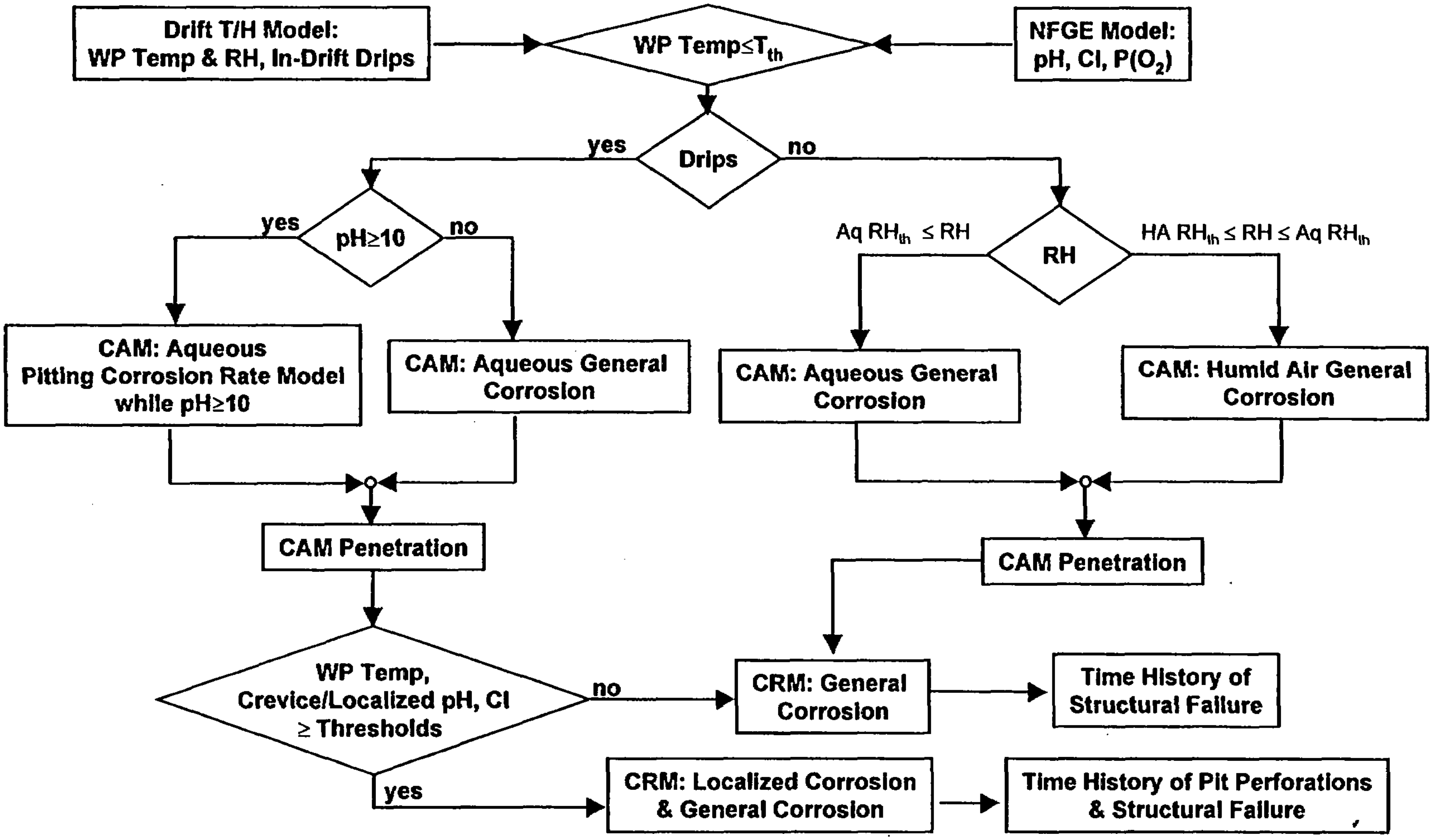
* pH, [Cl⁻] of dripping water, $P(O_2)$, across repository from NFE model



s - Patches with drips;
Potential salt deposits;
CRM localized corrosion

x - Patches with welds

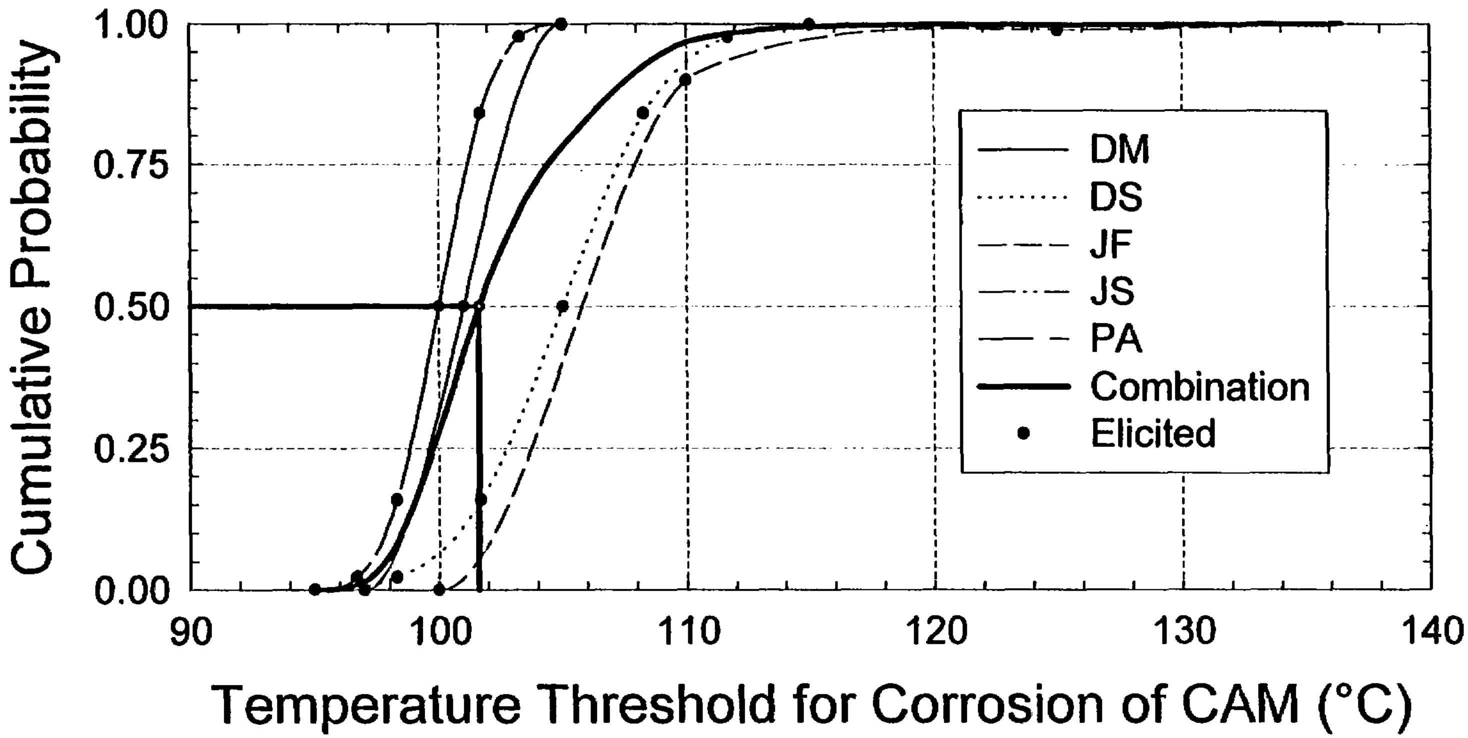
Logic Diagram for the Base Case TSPA-VA WP Degradation Model



Key Parameters for the TSPA-VA Base Case Waste Package Degradation Model

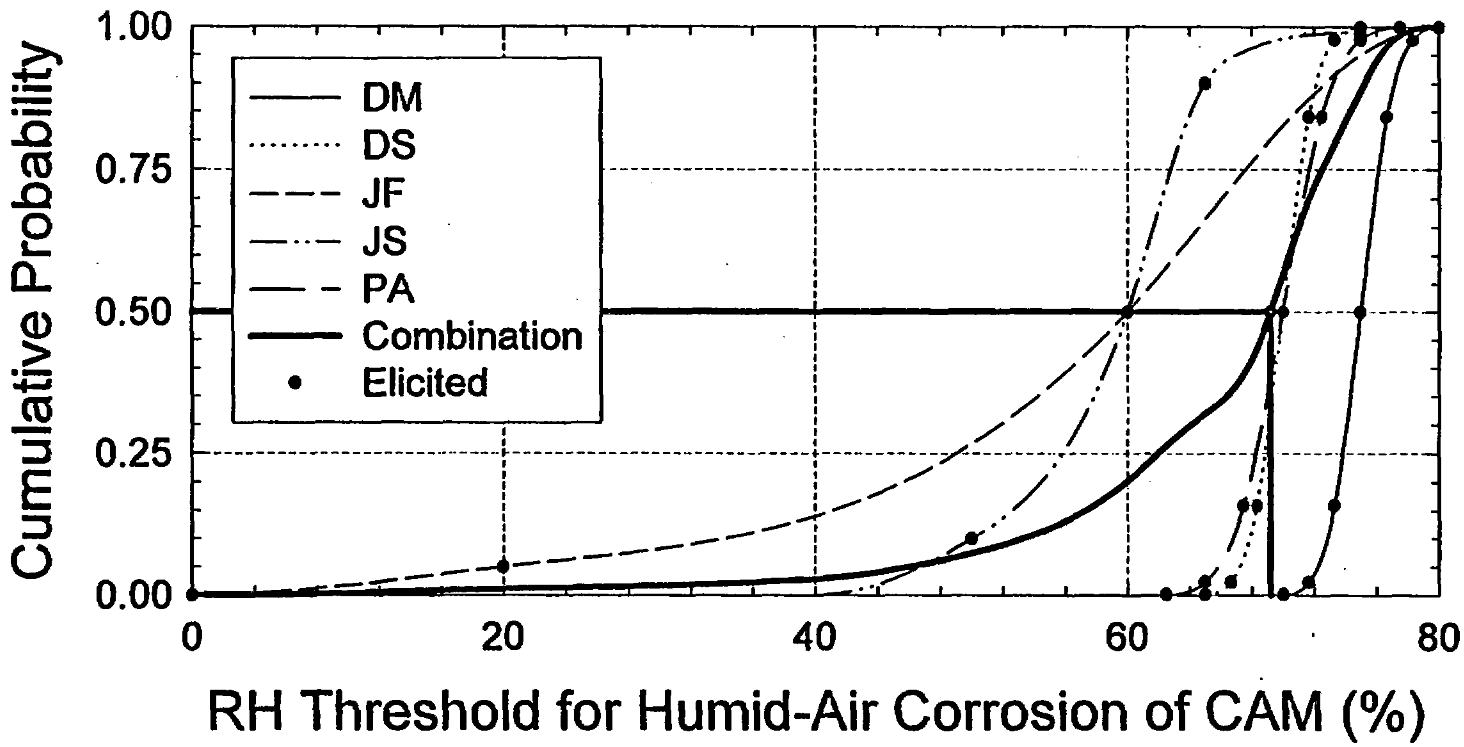
- Thresholds for CAM corrosion initiation
  - thresholds dependent on the surface condition (dust, oxides, salts), dripping, location on a WP (top, sides, bottom)
  - temperature threshold
  - RH threshold for humid-air corrosion
  - RH threshold for aqueous corrosion

Distribution for Temperature Threshold for CAM Aqueous or Humid Air Corrosion Initiation



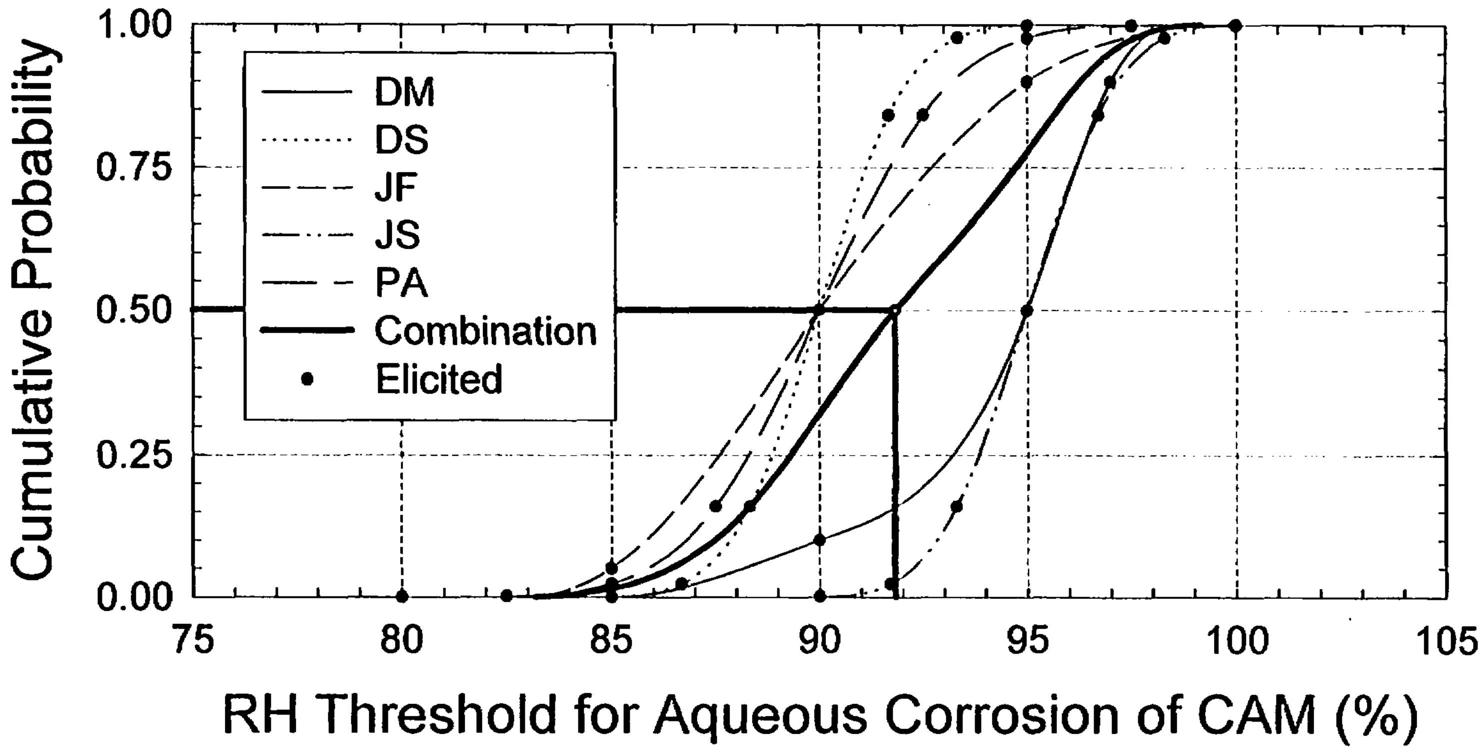
"Preliminary Draft"

Distribution for RH Threshold for CAM Humid-Air Corrosion Initiation



"Preliminary Draft"

Distribution for RH Threshold for CAM Aqueous Corrosion Initiation



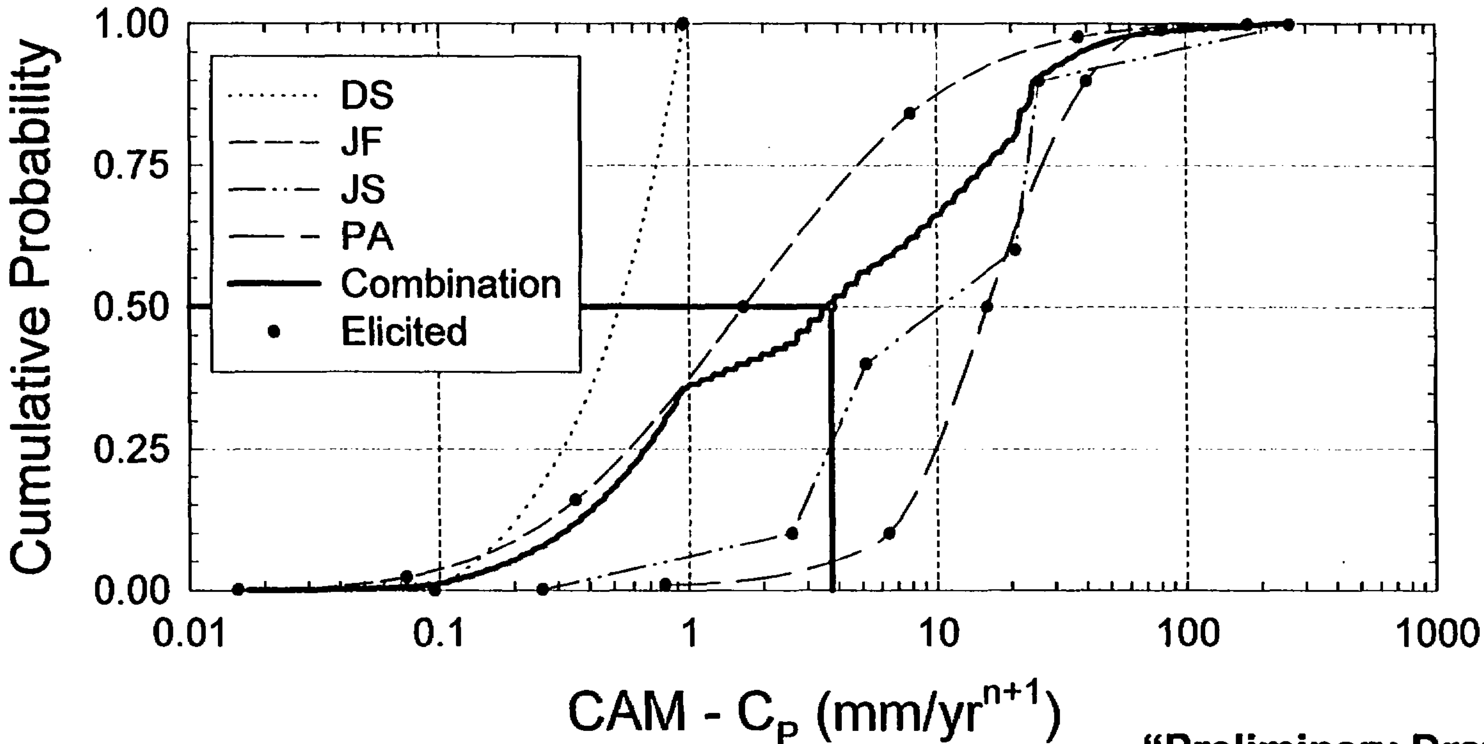
"Preliminary Draft"

Key Parameters for the TSPA-VA Base Case Waste Package Degradation Model

(continued)

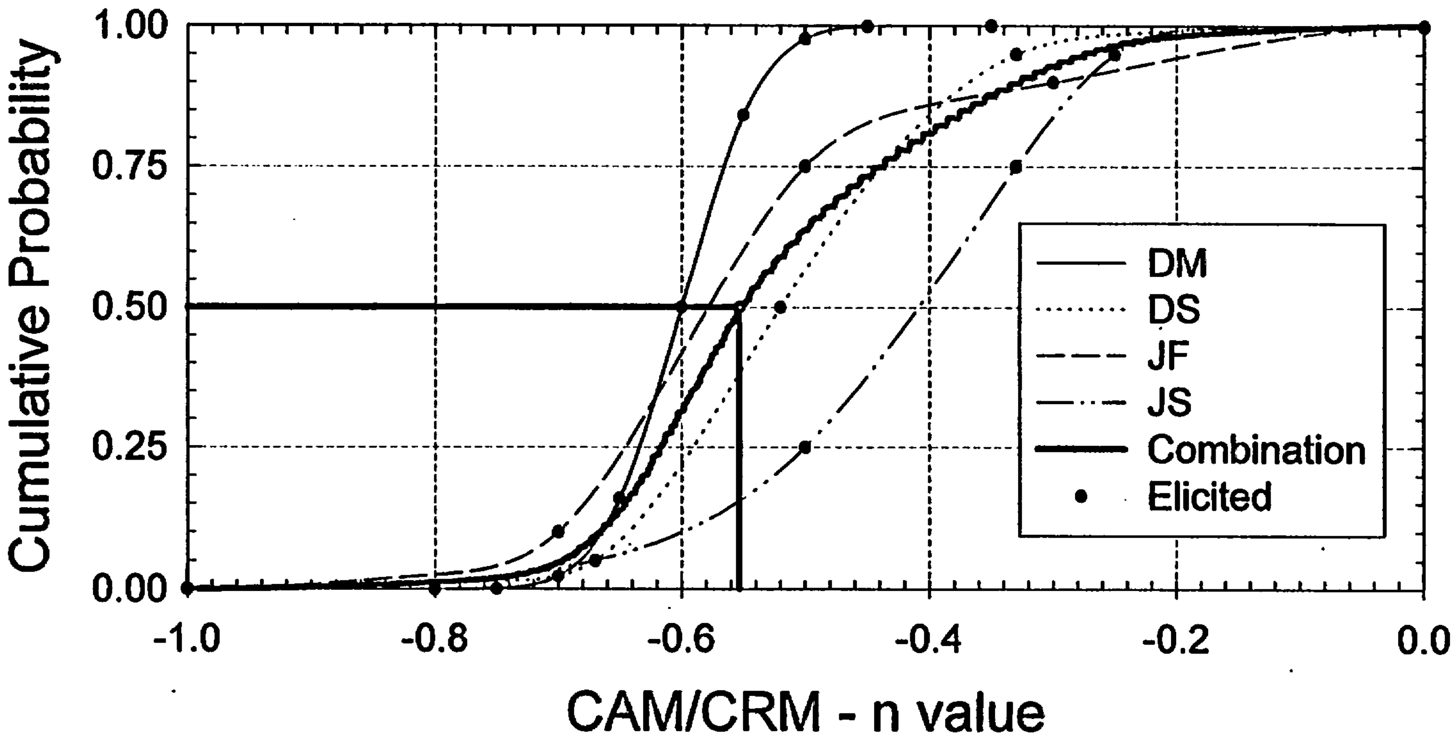
- CAM corrosion modes
  - humid-air or neutral pH (4 to 10) aqueous condition
    - » use TSPA-95 model for neutral pH aqueous general corrosion
    - » use TSPA-95 model for humid-air general corrosion
    - » general (uniform) corrosion with low localized variations
  - alkaline (pH≥10) aqueous condition
    - » high aspect ratio pitting model
    - » use pit growth law, rate = $R_G + C_P t^n$
      - R_G = general corrosion rate
      - C_P = constant for pit growth rate
    - » use "modified" TSPA-95 model for $R_G = f(t,T,pH)$
    - » pit density

Distribution for Constant 'C_P' of Pit Growth Rate (= $R_G + C_P t^n$) for CAM Pitting Corrosion in Alkaline Conditions (pH≥10)



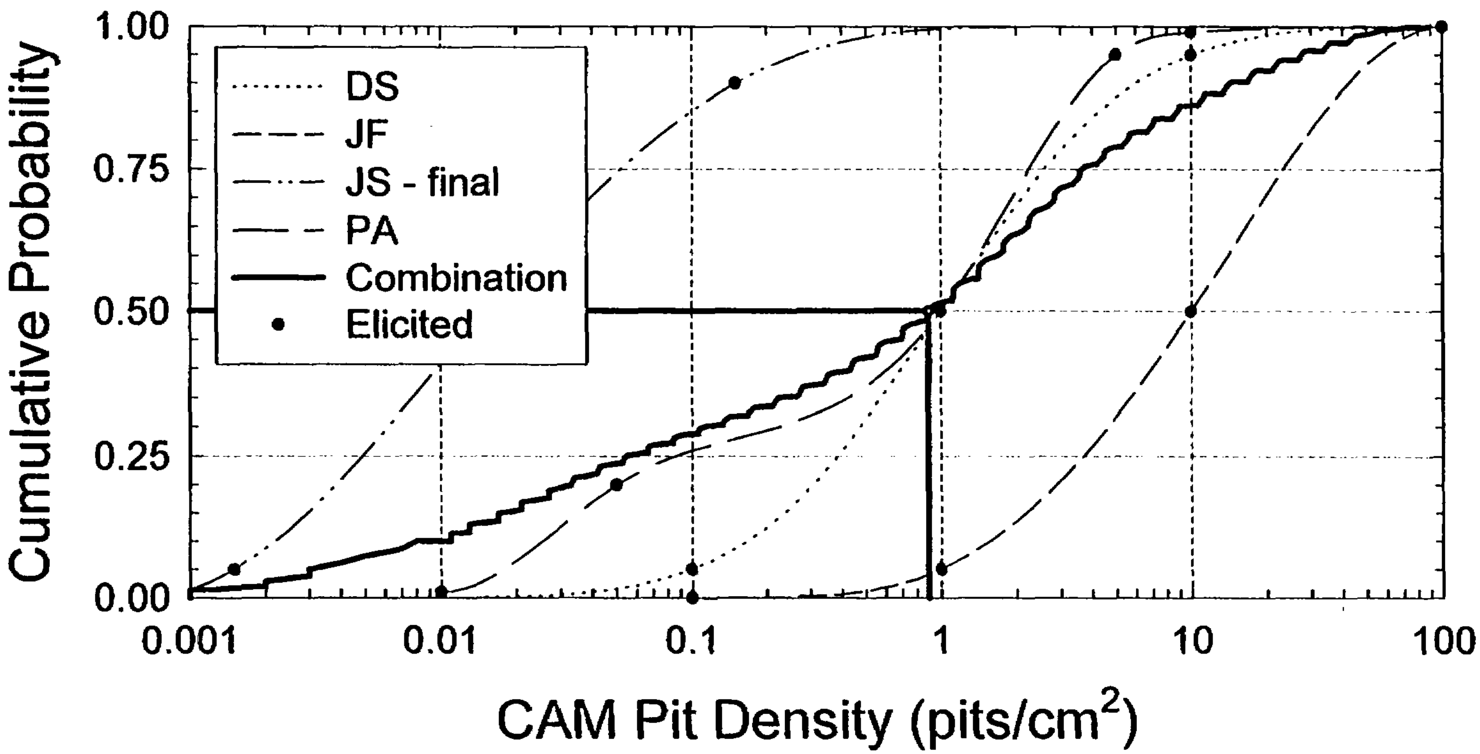
"Preliminary Draft"

Distribution for Constant 'n' of Pit Growth Rate (= $R_G + C_P t^n$) for CAM Pitting Corrosion in Alkaline Conditions (pH≥10)



"Preliminary Draft"

Distribution for Pit Density of CAM in Alkaline Conditions (pH≥10)



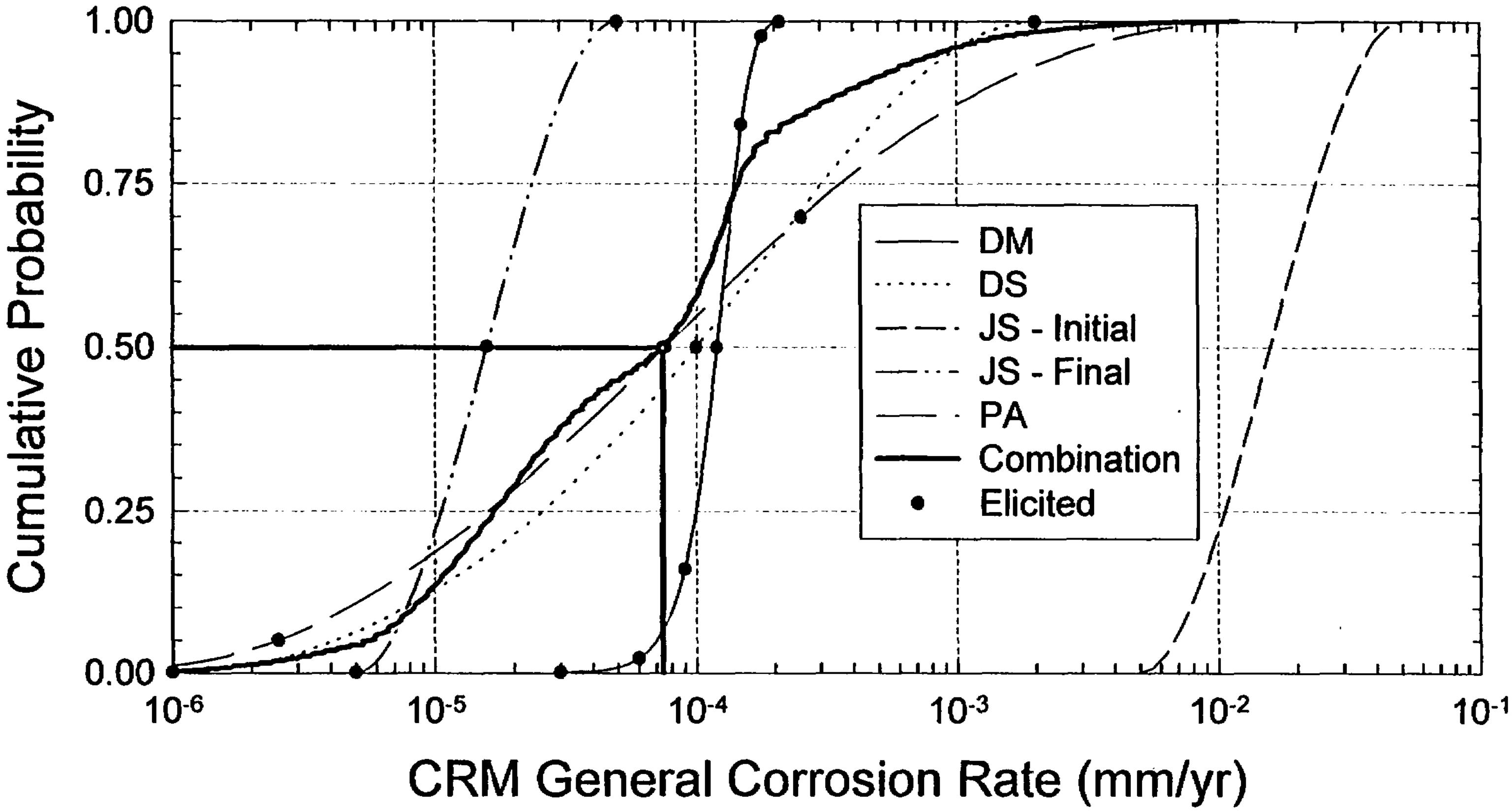
"Preliminary Draft"

Key Parameters for the TSPA-VA Base Case Waste Package Degradation Model

(continued)

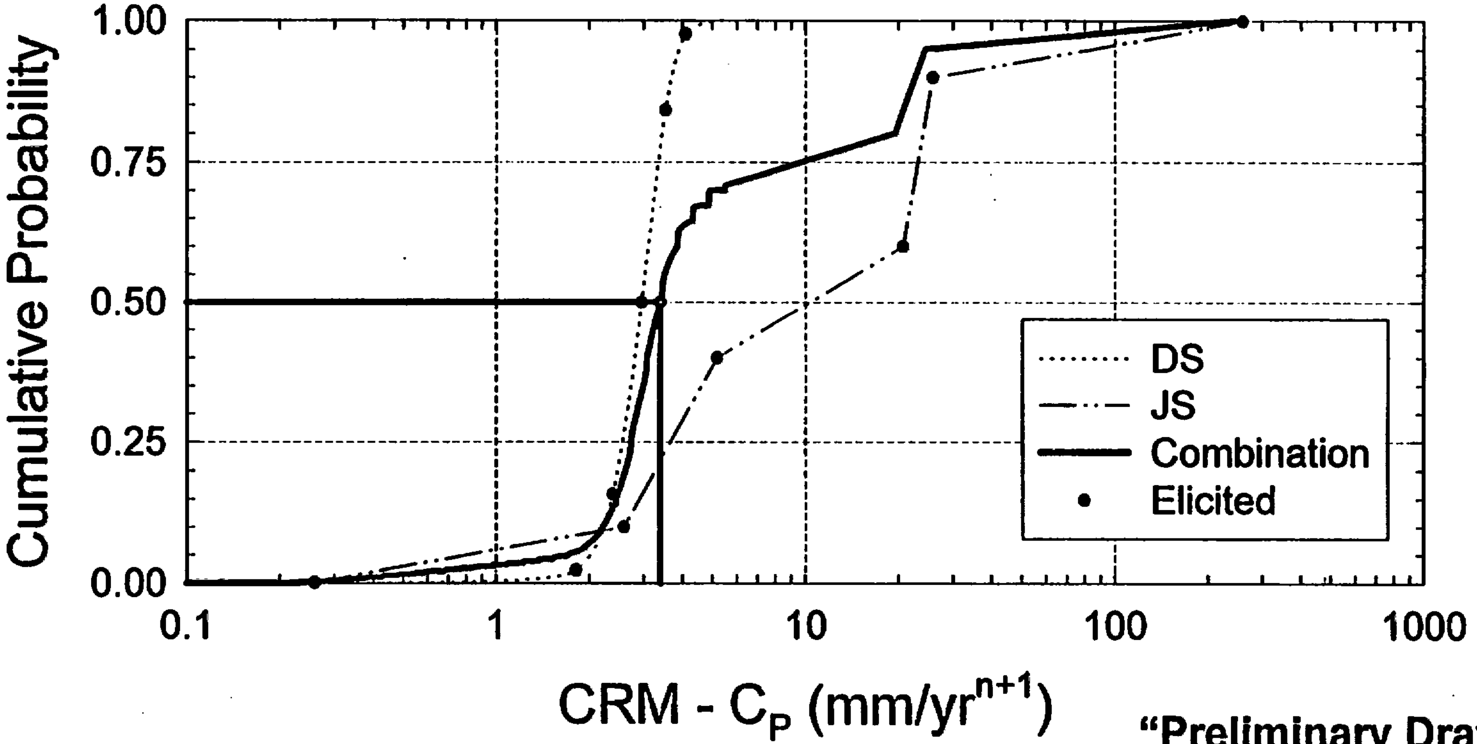
- CRM corrosion mode
  - general corrosion of CRM under humid-air or "non-dripping" aqueous condition
  - marginal galvanic protection of CRM (a few 100 years at most)
  - localized (pitting/crevice) corrosion requires drips with elevated Cl^- and low pH within a crevice and pit
  - use pit growth law for pitting and crevice corrosion
    - » pit growth rate = $R_G + C_P t^n$
      - R_G = general corrosion rate
      - C_P = constant for pit growth rate
    - » pit density and pit diameter

Distribution for Constant 'R_G' of Pit Growth Rate (= $R_G + C_P t^n$) for CRM Pitting/Crevice Corrosion



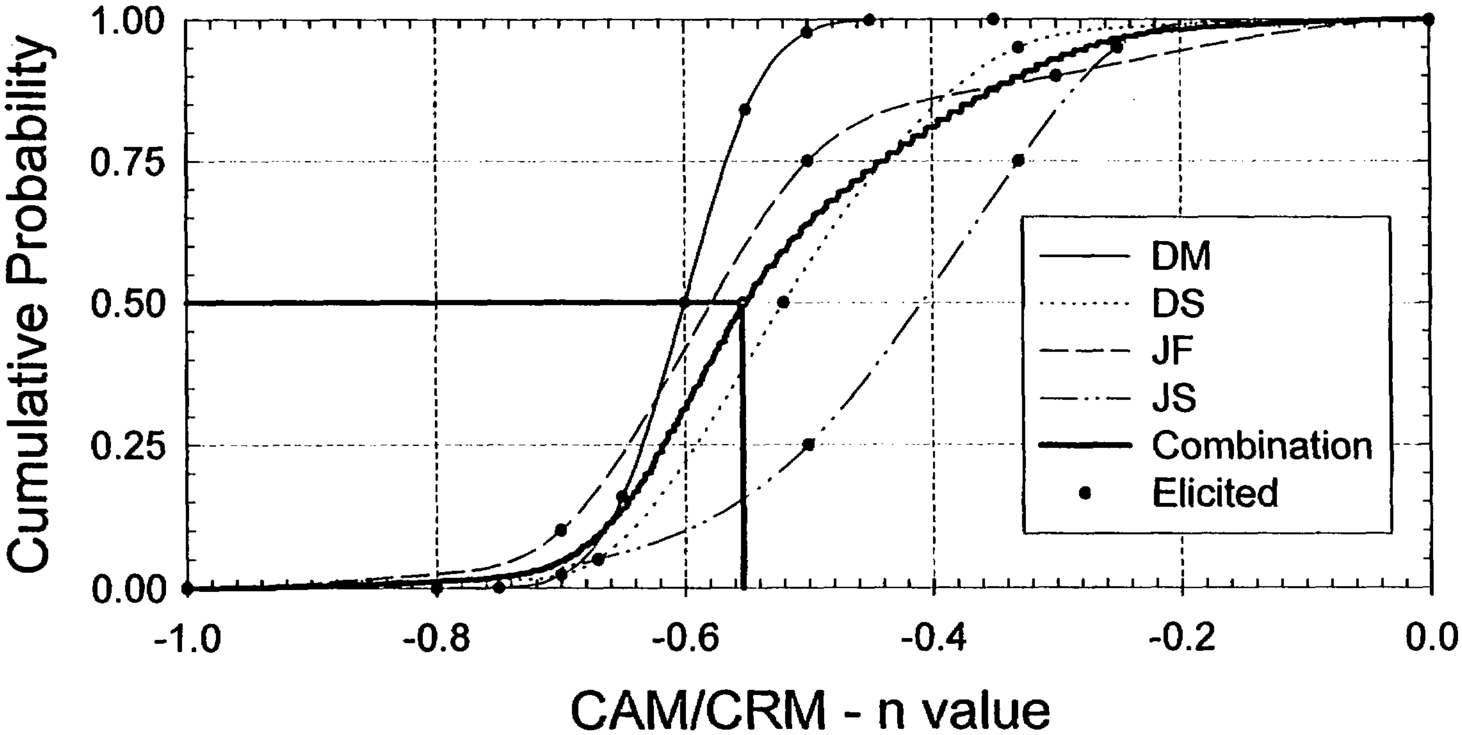
"Preliminary Draft"

Distribution for Constant 'C_P' of Pit Growth Rate (= $R_G + C_P t^n$) for CRM Pitting/Crevice Corrosion



"Preliminary Draft"

Distribution for Time Constant 'n' of Pit Growth Rate (= $R_G + C_P\, t^n$) for CRM Pitting/Crevice Corrosion



"Preliminary Draft"

Representation of Variability and Uncertainty in Waste Package Degradation

- Potential sources of variability in waste package degradation
  - WP materials, WP fabrication including welds
  - temporally and spatially varying (bulk) exposure conditions
    - » WP surface temperature, RH
    - » drip location, drip rate and frequency, drip water chemistry (particularly pH and Cl-)
    - » gas phase composition (particularly O_2 partial pressure)
  - variable local environments
    - » crevice formation between the barriers, under corrosion products and/or mineral deposits
    - » water chemistry within crevice and pit
    - » rockfalls

Representation of Variability and Uncertainty in Waste Package Degradation
(continued)

- Potential sources of uncertainty in waste package degradation
  - uncertainties in corrosion conceptual models and process models
  - uncertain exposure conditions
    - » drip location, drip rate and frequency, drip water chemistry (particularly pH and Cl-)
  - uncertain local environments
    - » crevice formation between the barriers, under corrosion products, and mineral deposits
    - » water chemistry within crevice and pit
    - » rockfalls

Representation of Variability and Uncertainty in Waste Package Degradation
(continued)

- Incorporate explicitly the effects of temporally and spatially varying exposure conditions
  - Temperature, relative humidity, in-drift water dripping
  - chemistry of dripping water (pH, Cl), oxygen partial pressure
- Development underway to represent the effects from other sources not explicitly accountable

Concluding Remarks

- The WPDEE results will be incorporated extensively in the TSPA-VA base case and sensitivity analyses
  - develop scenarios for the base case and sensitivity analysis
  - develop/derive key model parameters
- The base case and sensitivity analyses of waste package degradation modeling in TSPA-VA will be focused to evaluate the effect of waste package performance
  - waste containment and isolation
    - » time-history of waste package failure (first pit perforation)
    - » time-histories of waste package perforations
  - alternative options for waste package design
  - effects of alternative EBS designs

ATTACHMENT 17

NRC'S APPROACH TO WASTE PACKAGE DEGRADATION MODELING

by

Sitakanta Mohanty, Gustavo Cragnolino, Darrell Dunn, and Narasi Sridhar
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Nuclear Regulatory Commission
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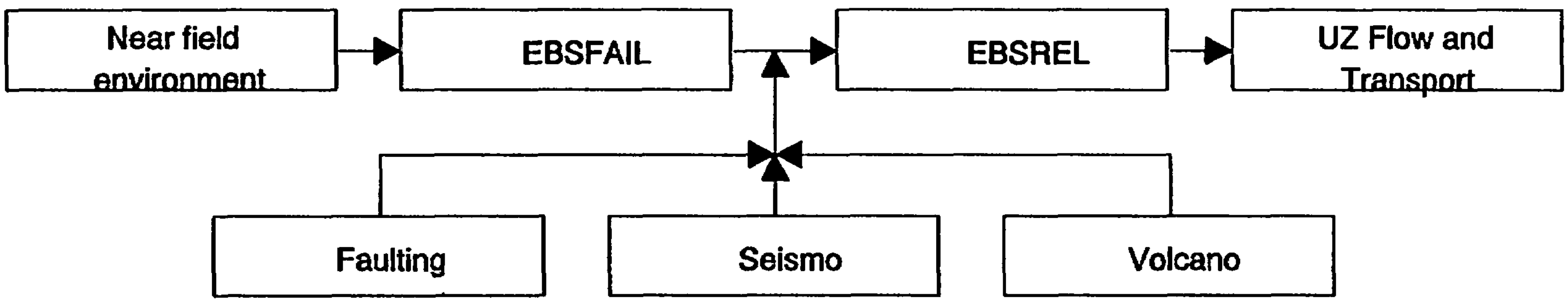
November 5-6, 1997
DOE/NRC Technical Exchange on
Total System Performance Assessments for Yucca Mountain

ENGINEERED BARRIER SYSTEM FAILURE (EBSFAIL) MODULE

- A consequence module of TPA Version 3.1 code



- A part of Engineering Barrier System Performance Assessment Code (EBSPAC) Version 1.1

- Calculates failure time of waste packages (WPs) due to various degradation modes including corrosion and mechanical processes

FAILURE OF WASTE PACKAGE IN EBSFAIL

- WP failure by corrosion is defined as through-wall penetration of outer and inner overpacks by a single pit or by uniform dissolution

- Modes of WP corrosion:

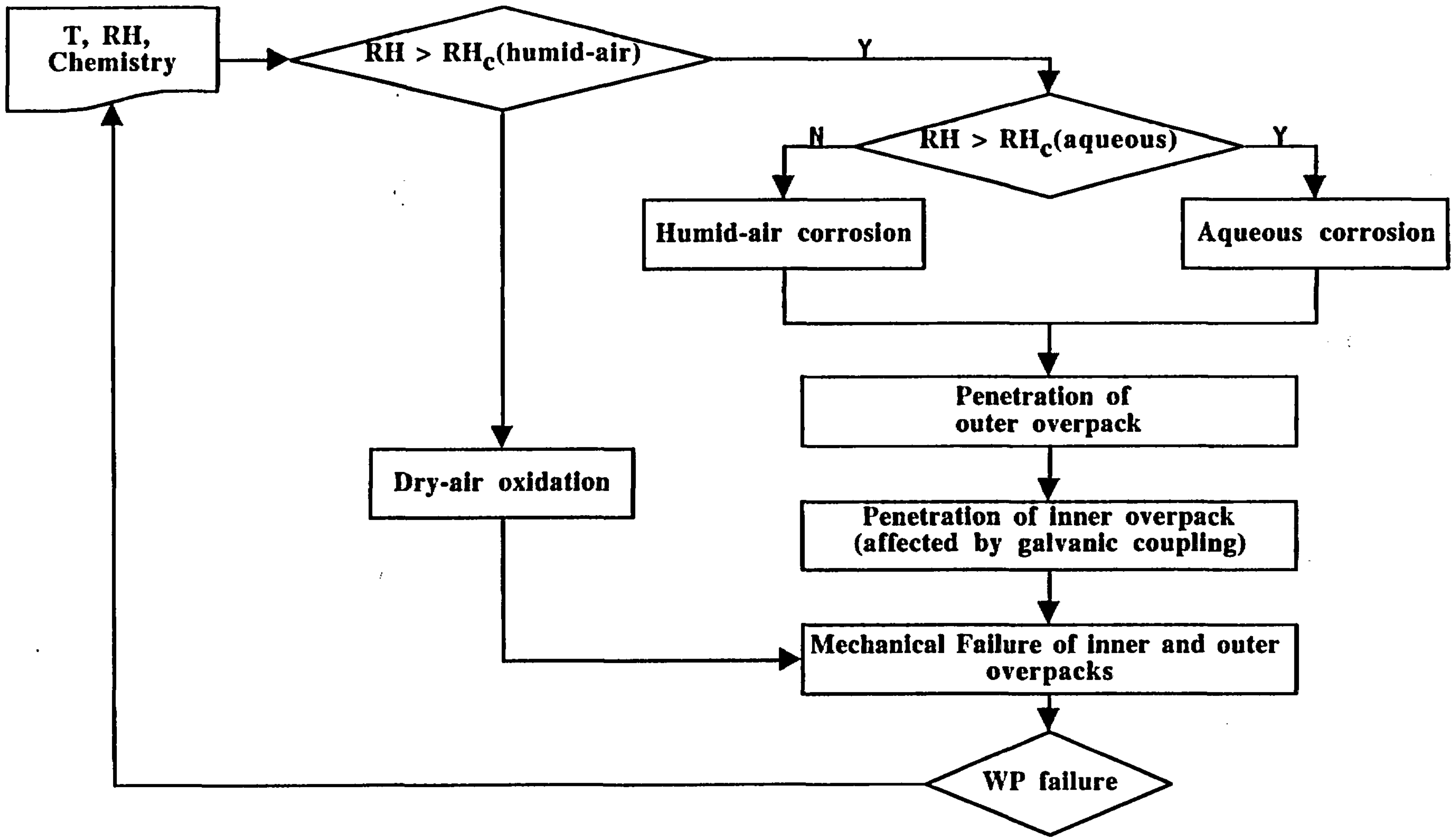
  - Outer overpack: air oxidation, uniform humid-air and uniform aqueous corrosion, and localized (pitting and crevice) aqueous corrosion

  - Inner overpack: uniform and localized aqueous corrosion

- WP failure can occur by brittle failure due to mechanically dominated processes resulting from fabrication stress

- WP failure can also occur from events modeled outside of EBSFAIL such as fault movement, seismic events, and volcanic events

PROCESS FLOW CHART FOR EBSFAIL



CONCEPTUAL MODEL APPROACHES

- WP corrosion affected by temperature, RH, and water chemistry at WP surface and evaluated using a combination of mechanistic modeling and experimentally measured parameters
  - Temperature based on a heat conduction model
  - RH calculated from water vapor pressure considering temperature difference between the WP surface and drift wall
  - Initiation of humid-air and aqueous corrosion determined by critical values of RH
  - Chemical composition of the aqueous phase with NaCl as the predominant soluble salt, including pH (as determined by [HCO_3]) and assuming a constant value equal to partial pressure of O_2 in air
- Mechanical failure of WP evaluated using a fracture mechanics approach

EVALUATION OF LOCALIZED AQUEOUS CORROSION

- **Corrosion potential:** $E_{corr} = f(T, pH, C_{O_2}, \ldots)$
- **Localized corrosion:** $E_{crit} = f(T, C_{CL^-}, material)$
- **Galvanic coupling:** $E_{WP}^{825} = (1-\eta)\ E_{corr}^{825} + \eta\ E_{couple} \qquad 0 \le \eta \le 1$
- **Conditions for Localized Corrosion**
  - Outer overpack: $E_{corr}^{A516} > E_{crit}^{A516} \qquad at\ pH > 9.0$
  - Inner overpack: $E_{WP}^{825} > E_{crit}^{825}$

LOCALIZED CORROSION PENETRATION RATES

- Maximum pit penetration rate for A516 steel [Marsh & Taylor. Corrosion Science. 28,289-320 (1988)]

$$\frac{dP}{dt}(mm/yr) = 3.897\ t^{-0.55}$$

- Pit penetration rate for Alloy 825

$$\frac{dP}{dt} = 0.18 \quad mm/yr$$

EVALUATION OF WP MECHANICAL FAILURE

- Stress intensity defined as

$$K_I = Y\sigma\ (\pi a)^{1/2}$$

where

Y = geometry factor, depends on crack shape and load configuration and incorporates a safety factor of 1.4

σ = applied stress, assumed to be equal to yield strength for residual stresses in welds

a = depth of the crack, assumed to be equal to pit depth

- Condition for mechanical failure

$$K_I > K_{IC}$$

where K_{IC} is the fracture toughness

DIFFERENCES BETWEEN EBSFAIL AND WAPDEG APPROACHES

EBSFAIL	WAPDEG
Combinations of mechanistic models and experimentally measured parameters using laboratory generated database	Empirical models for humid air and aqueous corrosion using parametric equations based on a limited field database (rural and urban atmospheres, lake and river waters)
Near-field chemistry considered	No consideration of near-field environment (except for T and RH)
Penetration by dry oxidation is continued through uniform or localized corrosion under wet conditions	Dry oxidation considered negligible
Mechanical failure of outer overpack by fracture	No mechanical failure considered

DIFFERENCES BETWEEN EBSFAIL AND WAPDEG APPROACHES

EBSPAC	WAPDEG
Penetration of a representative pit through both containers constitutes failure of the WP. No degradation history beyond the penetration of the representative pit	Penetration of the deepest pit from multiple pits, initiated simultaneously but grown stochastically, constitutes WP failure, but degradation continues
Empirical or process-based model for pitting corrosion based on experimentally measured or estimated growth rates	Pitting rate of outer overpack is calculated by multiplying uniform corrosion rate by a sampled factor. Pitting of the inner overpack is calculated from a temperature-dependent equation.
Corrosion failure of all WP in a subarea (SA) occur at the same time	Failure time distribution is due to variations in hydrothermal conditions at various locations.

UNCERTAINTIES IN EBSFAIL

- WP corrosion
  - Temperature of WP and critical relative humidity
  - Water chemistry (Chloride concentration, pH, Oxygen partial pressure)
  - Dissolution rate of alloys under passive and localized corrosion conditions
  - Effectiveness of galvanic protection
- Mechanical disruption of WP
  - Magnitude and location of stress/deformation fields
  - Changes in fracture toughness due to thermal embrittlement

ACTIVITIES FOR ASSESSING EFFECTIVENESS OF GALVANIC COUPLING

- Improve mechanistic understanding of galvanic coupling
- Develop methodology to estimate galvanic coupling efficiency
- Simplified modeling used in "An Analysis of Galvanic Coupling Effects on the Performance of High-Level Nuclear Waste Container Material", CNWRA 97-010, August 1997.
  - Geometry of galvanic couple defined by pit penetrating outer A516 steel container and exposing alloy 825 to local, acidified environment
  - Evaluation of the influence of environmental and electrochemical parameters, in addition to the effect of area ratio, on the efficiency of galvanic coupling
- Galvanic corrosion potential for alloy 825 as a function of galvanic coupling efficiency compared with critical potential to determine propensity to localized corrosion

ATTACHMENT 18

YUCCA MOUNTAIN PROJECT

Studies

Dilution of Radionuclide Concentration at a Pumping Well: Preliminary Implications for Performance Assessment

Presented to
DOE/NRC Technical Exchange on
Total System Performance Assessment
Las Vegas, Nevada

Presented by:
Bill W. Arnold, Senior Member Technical Staff
George E. Barr, Distinguished Member Technical Staff
Sandia National Laboratories
Albuquerque, New Mexico

U.S. Department of Energy
Office of Civilian Radioactive
Waste Management

November 6, 1997

Sandia National Laboratories

Dilution at a Pumping Well

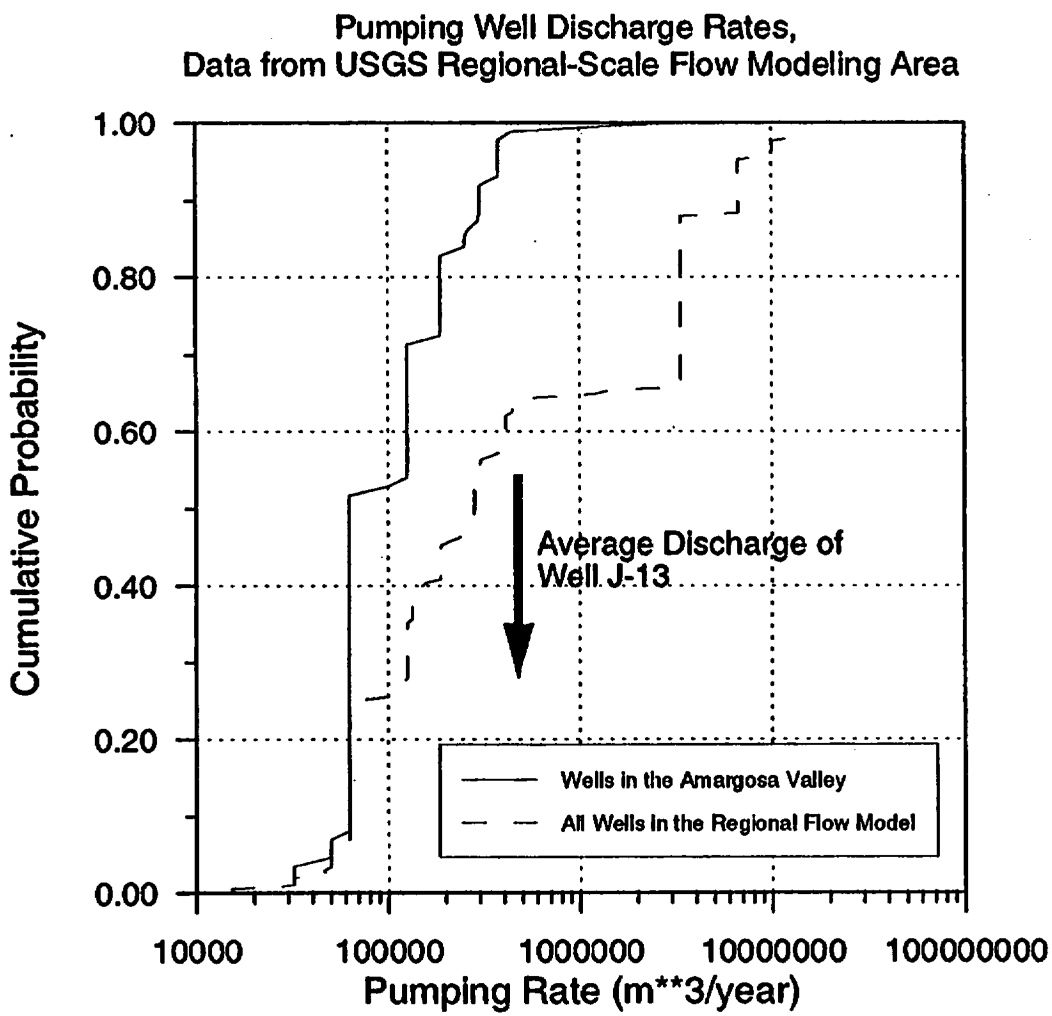
- Dilution of radionuclide concentration at a potential pumping well is expected to be influenced by:

  1) Pumping rate.
  2) Completion interval of well, screen length.
  3) Contaminant plume dimensions, width of the plume. Simulated plume width would be influenced by:
     - Dimensionality of the analysis.
     - Transverse dispersion.
     - Continuum vs. discrete fracture representation.
     - Time since initiation of the source.
     - Geometry of the source.
  4) Sorption.

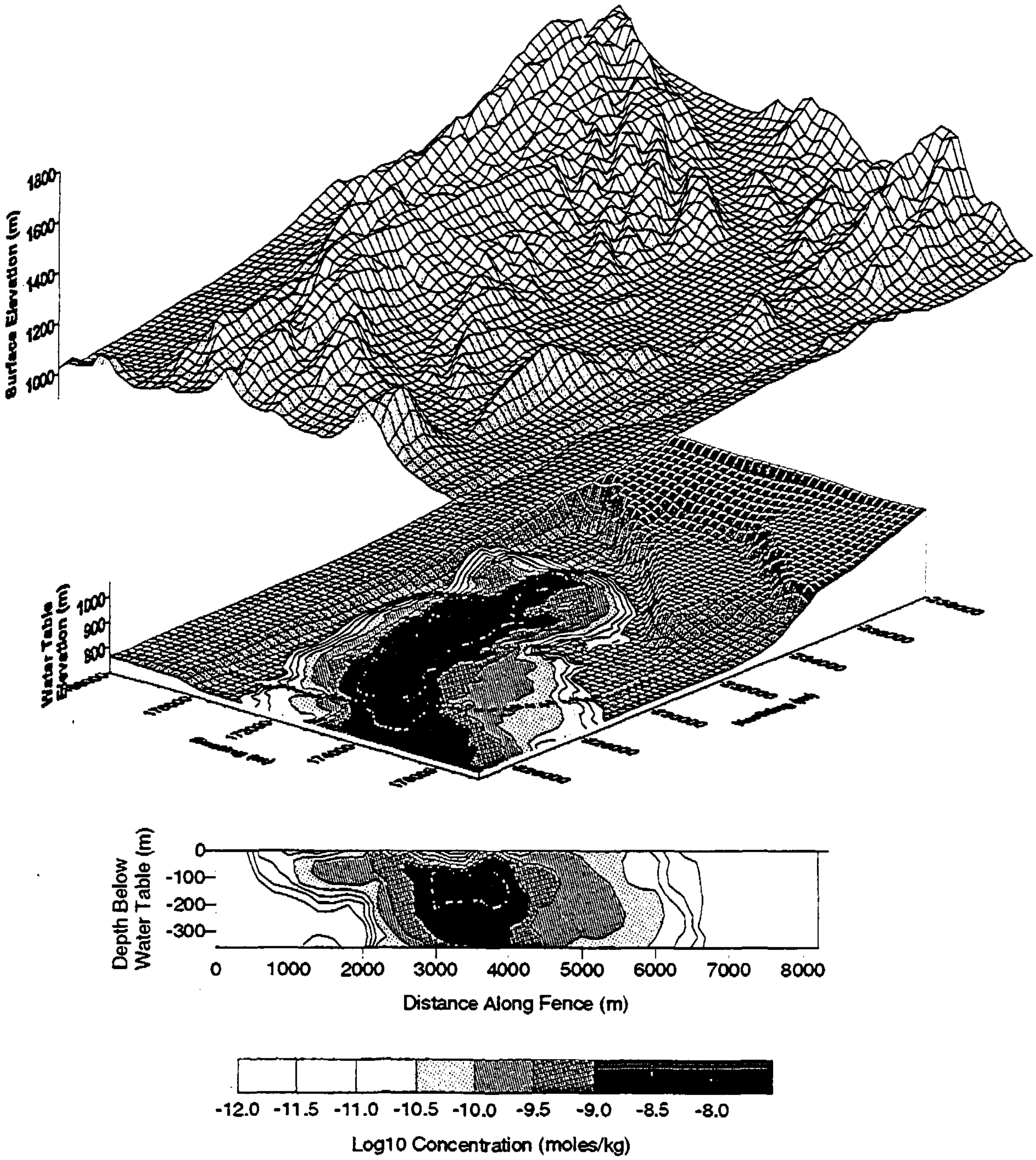
- A possible abstraction of dilution at a pumping well for TSPA analyses is to use a dilution factor based on reduction of radionuclide concentration at the well under steady-state pumping conditions (flow and solute transport).

Sandia National Laboratories

- **Present-day groundwater utilization patterns as guidance for potential future pumping.**

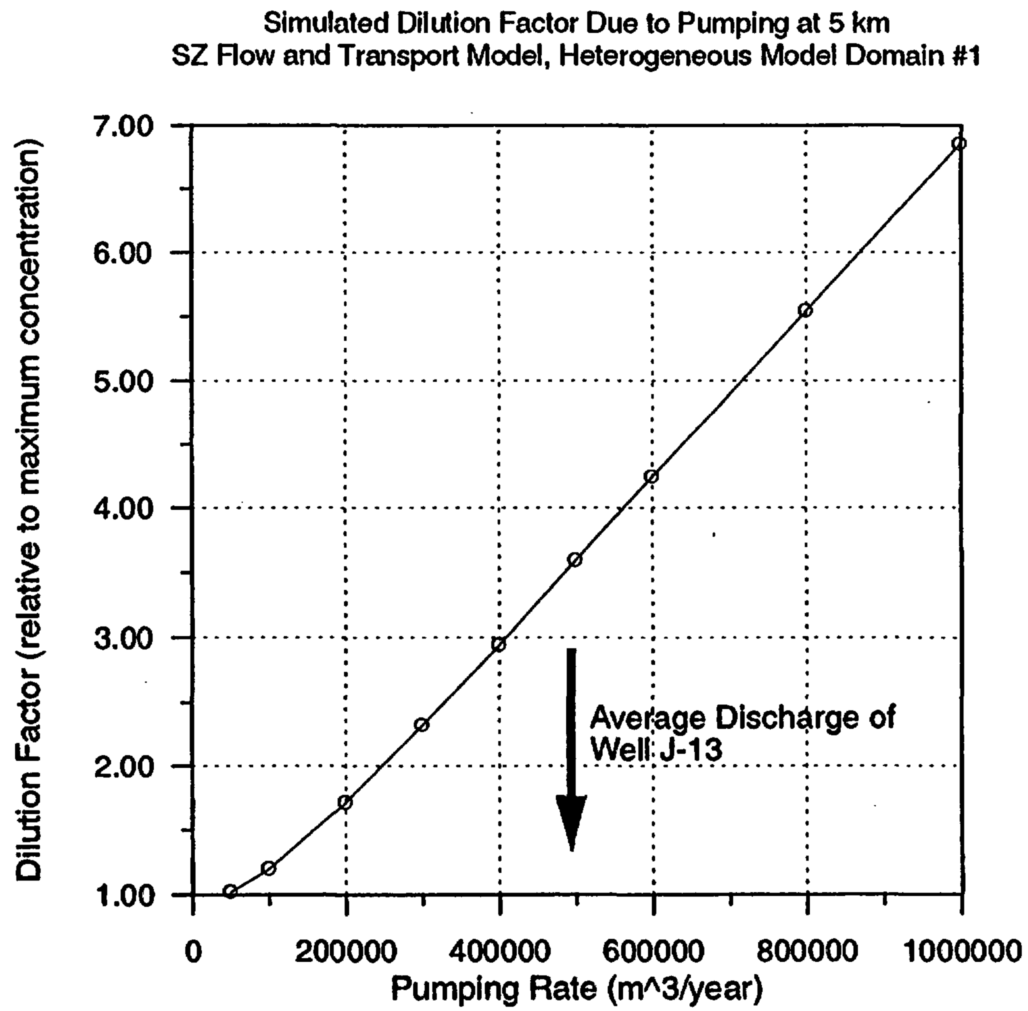


Three-Dimensional Groundwater Flow and Transport Model using FEHM
Heterogeneous Domain, Steady Solute Source of 1 mole/year at the Water Table Footprint of the Repository

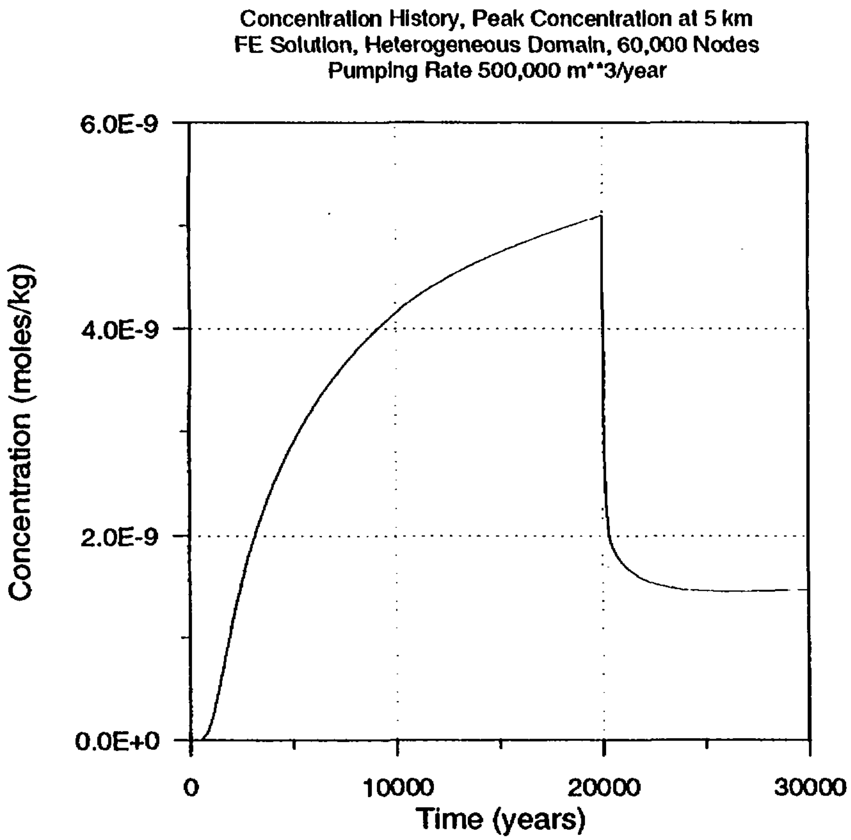


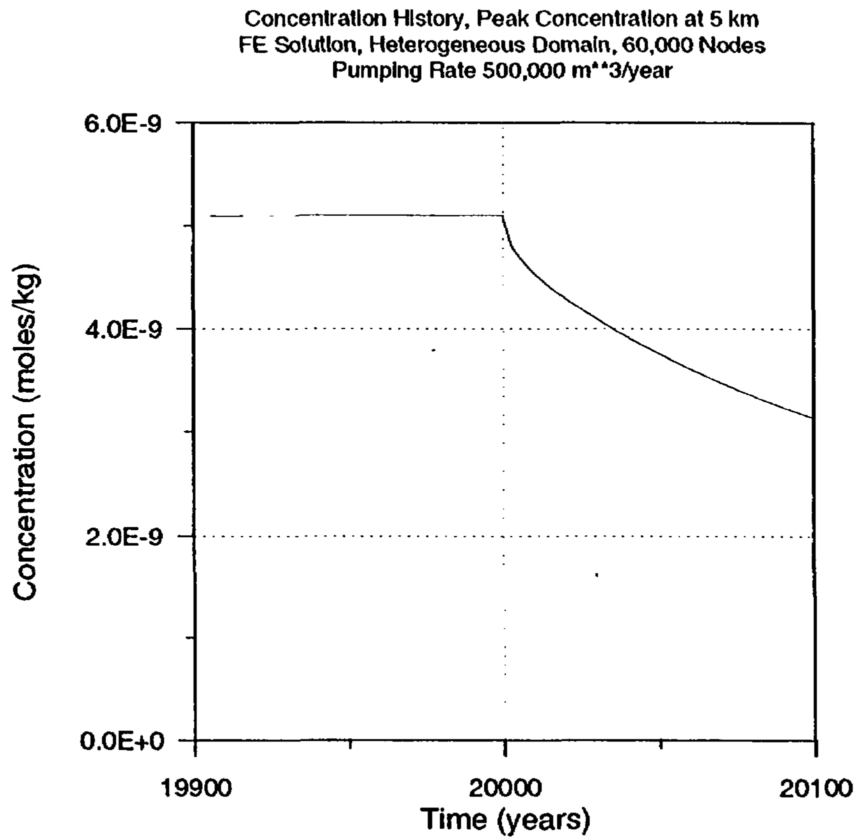
Sandia National Laboratories

- **Steady-state concentration reduction factor based on transport modeling of a conservative solute as a function of well discharge.**



• **Transient modeling shows that there may be a significant delay in reaching steady-state conditions relative to the scale of human lifespan.**





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Implications for TSPA

- Assessment of radionuclide dilution at a pumping well for TSPA should be consistent with the SZ flow and transport simulation method used in TSPA analyses.
- For typical present-day well pumping rates in the Amargosa Valley and based on example 3-D flow and transport modeling, the steady-state well dilution factor for a conservative solute is small (1 - 3).
- The transient response (in terms of solute transport) of the system to a pumping well should be considered in calculating dilution. If time periods on the order of decades are required to achieve significant additional dilution at the well, then it may be prudent to disregard the effects of well dilution in TSPA analyses.

ATTACHMENT 19

EFFECT OF WASTE PACKAGE FAILURE ON RADIONUCLIDE RELEASE RATE

NOVEMBER 5-6, 1997
DOE/NRC TECHNICAL EXCHANGE ON
TOTAL SYSTEM PERFORMANCE ASSESSMENTS FOR YUCCA MOUNTAIN

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PERFORMANCE ASSESSMENT AND HLW INTEGRATION BRANCH
DIVISION OF WASTE MANAGEMENT

Premise: Radionuclide release depends strongly on mode of waste package failure

1. Mode of failure determines how water will enter and leave

2. Mode of failure will affect chemistry inside waste package

3. Corrosion products might limit flow and diffusion to outside of waste package

4. Corrosion product may serve as effective sorbers of released radionuclides both inside and outside the waste package

1. Mode of failure determines how water will enter and leave the canister

A. "Bathtub" model

- Water enters canister in one corrosion hole and leaves through the same or a different hole.
- Height of water in bathtub determined by the position of the holes
- Bathtub can involve a large fraction of the fuel by immersion
- Bathtub might be transient; exist for several thousands of years until other corrosion holes cause it to empty. "Pulling the plug" Might lead to a transient increase in release rate

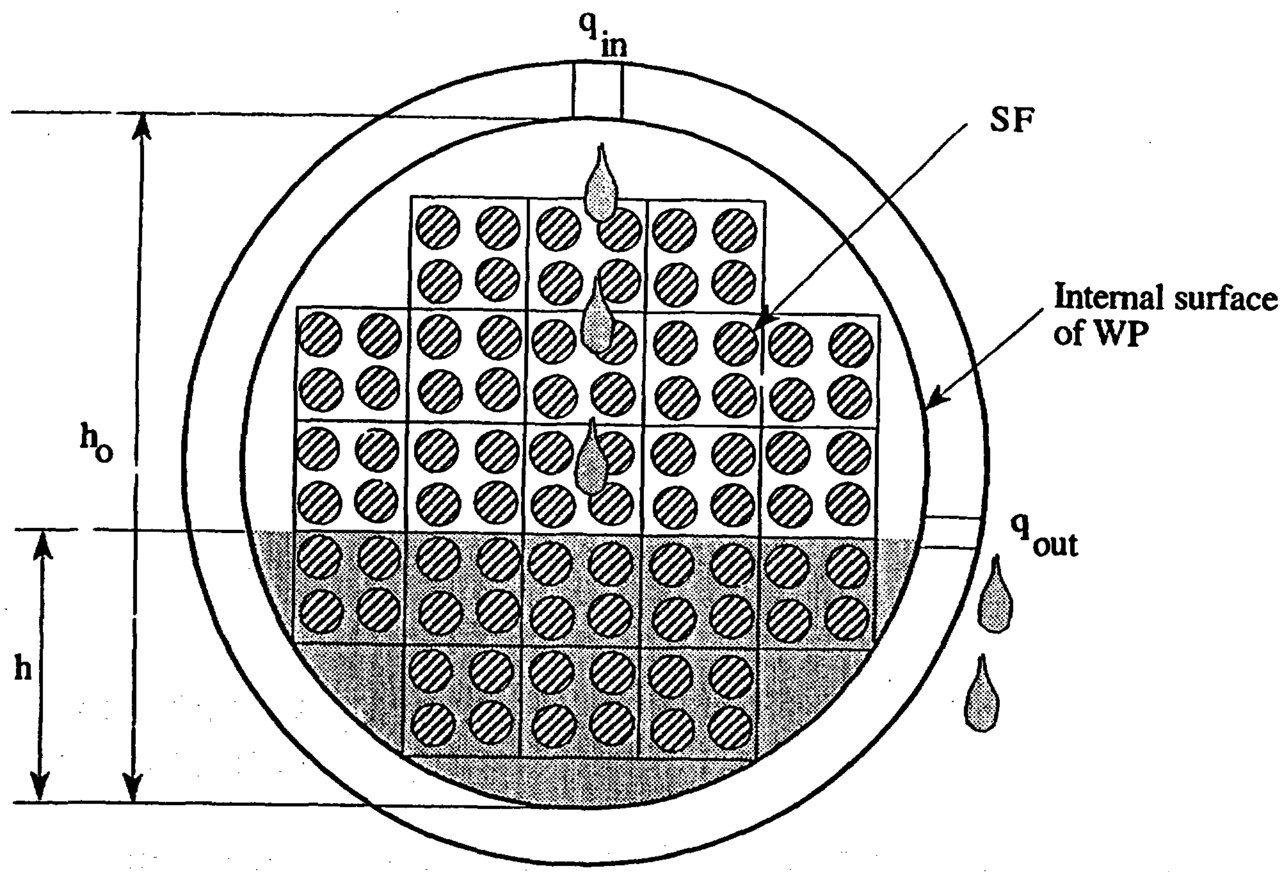


Figure 2-8. Schematic of the bathtub concept inside the waste package. Water encroachment (q_{in}) and withdrawal (q_{out}) points on the horizontally emplaced waste package are chosen to be on the top and side, respectively.

B. Flow-through model

- Water enters and leaves canister by corrosion holes, But does not pool
- Smaller portion of fuel involved; only that portion wetted by dripping water or water vapor inside canister, *but*
- Dripping water could be more corrosive of fuel per unit wetted area than stagnant water

2. Mode of failure will affect chemistry inside Waste package

- Corrosion of waste-package and waste-form materials will consume oxygen and possibly other constituents entering the waste package (e.g., silica)

- Size and properties of corrosion holes might limit the easy exchange of atmospheric oxygen. Reduced partial pressure of oxygen will likely reduce release rates of many radionuclides.

3. **Corrosion products might limit flow and diffusion to outside of waste package**

- Area of corrosion holes and properties of filling material will affect advective and diffusive transport of radionuclides
- Low pH inside corrosion pit might limit amount of iron oxide precipitate

4. **Corrosion product may serve as effective sorbers of released radionuclides both inside and outside the waste package**

Conclusions

- Mode of waste package failure will affect release of radionuclides
- There can be substantial credit for waste package components even under failed conditions, but their use must be justified.

ATTACHMENT 20

YUCCA
MOUNTAIN
PROJECT

Studies

The "Biosphere" Food Consumption Survey

Presented at:
NRC/DOE Total System Performance Assessment Technical Exchange

Presented by:
David A. Swanson, Ph.D.

Yucca Mountain Site Characterization Office

U.S. Department of Energy
Office of Civilian Radioactive Waste Management

November 6, 1997

The Biosphere Food Consumption Survey

I. Background

II. Goals of the Full Survey

III. Characteristics of the Full Survey

IV. Data Quality and File Development Steps

V. Uses to-Date and Current Developments

VI. Discussion Issues

I. Background

Amargosa Valley Pilot Study conducted January-February, 1997

- No quantitative figures existed on the level of consumption of locally produced food in the study area so M&O's socio-economic group designed a pilot study with two major goals, for which data were collected by UNLV's Cannon Center For Survey Research in January-February, 1997 using Computer Assisted Telephone Interviewing (CATI)

- Goal 1. With a random sample of n=55, the pilot revealed that locally produced food was consumed in 76 percent of all households in Amargosa Valley (95% certain that it is consumed in at least 63 percent of households). This indicated that a full survey should be done.

- Goal 2a. Identified a suitable Sample Frame for a survey of the entire 80 km circle

- Goal 2b. Identified a suitable instrument for a survey of the entire 80 km circle (hypothesis tests involving selected criteria and 16 alternative instruments in pilot)

- Goal 2c. With only 24 refusals, Cooperation Rate was very high (69% = [55/(24+55)]*100)

- Goal 2d. No strong community, food group, or frame bias but a need for Spanish language version of questionnaire and Spanish speaking interviewer

- Recommended use of inverse gradient sample design with following target sample sizes by area: Amargosa Valley, 280; Beatty, 300; Indian Springs, 50; Pahrump, 500.

- Need for specific food & water consumption information to calculate annual consumption of locally-produced food.

II. Goals of The Full Survey

- Measure the annual amount of water and locally-produced food, (in 11 categories), consumed by adults residing in the study area that can be used for input to GENII-S. Also capture additional information that may be needed for GENII-S Input (e.g., swamp cooler use) and provide estimates of precision (sample error) for data obtained from the survey.

- Measure demographics of adults residing in the 80 km circle study area, The study area includes Amargosa Valley, Beatty, Indian Springs, and Pahrump.

- While maintaining respondent confidentiality, collect data so that consumption, demographics, & geography can be linked and jointly measured for subsets of the adult population, one or more of which may serve as an empirically-based "critical group."

III. Characteristics of the Biosphere Food Consumption Survey

- A full-scale sample survey that was approved by OMB (#1910-1400) in April and subsequently conducted using CATI system at UNLV.

- A stratified random design insured an efficient sample, for which sample error was both measurable and minimal, given the resources available.

- Using information gained from pilot study, careful questionnaire design and interviewing procedures, thorough interviewer training, close supervision of interviewers, and CATI system, were used to minimize non-sampling error.

- 1,079 Interviews completed in early June, with n = 195 in Amargosa Valley; n = 250 in Beatty; n = 65 in Indian Springs; and n = 569 in Pahrump.

- 21 Spanish language interviews completed.

- Special "Difficult To Interview" sample (n=33) collected to determine if "non-response bias" was present and if special adjustments would be needed.

IV. Data Quality & File Development Steps

Data Quality Control & Non-Response Assessment

- 1st stage: Initial quality control checks
- 2nd stage: Descriptive statistics & "logical" checks
- 3rd stage: Assessment of non-response bias through comparison of "difficult to interview" respondents with other respondents

Weighting & Consumption Calibration

- 4th stage: Appropriate weights identified & in place
- 5th stage: Food consumption calibration

Food Consumption, Linkage & Confidentiality Assurance

- 6th stage: Individual & aggregate estimates of AAC, completed, population, geography, and food consumption linked
- 7th stage: Grid Cell matching for Amargosa Valley
- 8th stage: Respondent ID detached (Confidentiality assured)

Final File Construction & Documentation

- 9th stage: final documentation, EBF construction, and report on results, to be completed in September

Data Quality Control: Non-Response Assessment

Are those who refused or otherwise did not respond different from those who did? This question is important because of the potential for "Non-response Bias" in a survey.

$$\text{Non-response Bias} = B(\bar{y}_r) = \bar{Y}_r - \bar{Y} = \bar{M}(\bar{Y}_r - \bar{Y}_m)$$

Where	$\bar{y}_r$	=	Respondent sample mean
	$\underline{B}(\bar{y}_r)$	=	Bias of respondent sample mean
	$\underline{Y}_r$	=	Respondent Population mean
	$\underline{Y}$	=	Population mean (respondents plus non-respondents)
	$\underline{M}$	=	Proportion of non-respondents in the Population
	Y_m	=	Non-respondent Population mean

To answer this question we used highly skilled interviewers to "convert" a random sample of those who initially refused to be interviewed or were extremely hard to contact (9 or more attempts). This sample (n=33) was termed the "difficult to interview" group.

Statistical tests were conducted to see if response patterns for key questions differed between the "difficult to interview" group and the "not difficult to interview" group. This was done to see if special weighting or adjustment was needed for "non-response."

Using the formula given earlier, we are testing to see if $\bar{Y}_r$ is different from $\bar{Y}_m$ (or some equivalent parameter such as the proportion who answer "yes")

Ho: $\bar{Y}_r = \bar{Y}_m$ Ha: $\bar{Y}_r \neq \bar{Y}_m$ $\alpha = .05$

We found in virtually every test that we could "not reject Ho" and, therefore we assume that $\bar{Y}_r = \bar{Y}_m$

Conclusion: Non-respondents, on average, are not different than respondents. This finding made "weighting" much less complex than it would have been had the response patterns been different.

Example Statistical Test for Non-Response Assessment Table 1

Are the response patterns of the "difficult to interview" different from those "not difficult to interview"?

The example uses question no. 3 "....Have you eaten any locally produced food in the past year?"

Consumed Local Food?

Interview Type	YES	NO	Total
Not difficult to Interview	60.4% (612)	39.6% (401)	100.0% (1,013)
Difficult to Interview	65.6% (21)	34.4% (11)	100.0% (32)
Total	60.6% (633)	39.4% (412)	100.0% (1,045)

Chi-Squared Statistic = .35 (df = 1), p = .55, do not reject H_o.

Conclusion: The response pattern of the "difficult to interview" is not different from those "not difficult to interview." Assume that $\bar{Y}_r = \bar{Y}_m$

Area Weighting Data
Table 2

Sample and Total Household Frequency by Community
1997 Biosphere Survey

Community	Number of households surveyed n_h	Total number of households N_h	% of households surveyed
Amargosa Valley	195	452	43%
Beatty	250	751	33%
Indian Springs	65	529	12%
Pahrump	569	4,993	11%
Total	1,079	6,725	16%

* The sample is randomly drawn from households within each community.

Gender Weighting Data
Table 3

Sample and Total Frequency of Females by Community
1997 Biosphere Survey

	Sample*		Total*
Community	p_{hf}	p_{hf}/p_h	P_{hf}/P_h
Amargosa Valley	120	.615	.490
Beatty	151	.604	.435
Indian Springs	42	.646	.490
Pahrump	373	.656	.502

* The sample is randomly drawn from households within each community

Gender, Area, and Total Weights By Community
Table 4

Community		Weight Gender	Weight Area	Weight Total
Amargosa Valley	Male	1.32	.369	.487
	Female	0.80	.369	.295
Beatty	Male	1.424	.484	.689
	Female	.722	.484	.349
Indian Springs	Male	1.435	1.323	1.898
	Female	.762	1.323	1.008
Pahrump	Male	1.444	1.406	2.030
	Female	.761	1.406	1.078

Area Weight = $(1{,}079 * N_h / N) / n_h$

Female Weight = $(p_h * P_{hf} / P_h) / (p_{hf})$

Male Weight = $(p_h * P_{hm} / P_h) / (p_{hm})$

Total Weight = (area) * (gender)

Food Consumption Estimation Method

$$AAC_{ij} = (DPY_j)(CADI_i)(Q_{ij}) = (DPY_j)(Q_{ij})(ADI_i)/(FPC_i).$$

Where AAC_{ij} = annual amount of locally produced food *i* consumed by individual *j*

And $(CADI_i)$ = contingent average daily intake of food *i* (USDA survey)

= $(ADI_i)/(FPC_i)$

where ADI_i = average daily intake of food *i* (USDA survey)

and FPC_i = fraction consuming food *i* per day (USDA survey)

And Q_{ij} = locally produced fraction of total consumption during the months in which respondent *j* consumed locally produced food *i*: 1, 0.75, 0.5, or 0.25 as translated from "all," "most," "some," and "very little," *j's* response to 4th part of food question *i*

DPY_{ij} = number of days per year that *j* consumed locally produced food *i* = $DPW_{ij}*WPY_{ij}$

DPW_{ij} = (Days Per Week) = *j*=s response to 3rd part of food question *i*

WPY_{ij} = (Weeks Per Year) = $MPY_{ij}*(4.33)$

where MPY_{ij} = (Months Per Year) = *j*=s response to 2nd part of food question *i*

and 4.33 = average number of weeks per month over a year.

Example Food Consumption Question

3K1. Over the past year, did you eat any locally-produced eggs, including those from chickens, ducks, or other fowl, whether raw, or cooked in any way?

Yes
No
Don't Know
Refuse

3K2. Over how many months last year would you say you ate locally-produced eggs? Was it...

1-3 months
4-6 months
7-9 months
10-12 months
Don't know
Refuse

3K3. During those months in which you ate locally-produced eggs over the past year, about how many days per week would you say that you ate any?

Less than one day per week
1-2 days per week
3-4 days per week
5-6 days per week
7 days per week
Don't know
Refuse

3K4. During those same months, about how much of the TOTAL AMOUNT of eggs you ate was locally-produced? Would you say it was all, most, some or very little?

All
Most
Some
Very Little
Don't Know
Refuse

USDA Contingent Average Daily Intake for Adults
Table 5

	leaf	root	grain	fruit	poultry	beef	pork	game	fish	milk	eggs
male	179	150	308	318	147	134	72	143	105	408	100
female	137	114	217	293	103	104	58	67	116	301	71

from USDA 1987-88 "west" classification in:
USDA. 1993. Food and Nutrient Intakes by Individuals in the United States, 1 day, 1987-88.

* Measured in grams. Given that an adult (age 20 years and over) consumed the food in question, the table shows the amount consumed.

Example Food Consumption Calculations

Example 1. A female respondent ate locally produced fruit 3-4 days per week over 4-6 months during the year. Over the 4-6 months, "some" of the fruit she ate was locally produced. Her annual amount consumed (AAC) is calculated as:

AAC = (DPY)(CADI)(Q)

= (3.5*5*4.33)(293)(0.5)

= 11,101 gr.

= 11.101 kg.

Example 2. A male respondent said that he ate locally produced eggs 4-6 days per week over the entire year and that all of the eggs he consumed were local. His annual amount consumed (AAC) is calculated as:

AAC = (DPY)(CADI)(Q)

= (5.5*11*4.33)(100)(1.0)

= 26,197 gr.

= 26.20 kg.

Working Definitions For Three Different "Per-Adult" Consumption Levels

1. "**Subsistence**" = Those reporting that all of the food in question, "X," they consumed was locally produced

"Subsistence" per-adult consumption =

$$\frac{\text{(Amount consumed of Locally produced "X" by those only eating locally produced "X")}}{\text{Those only eating locally produced "X")}}$$

2. "**Partial Subsistence**" = "Subsistence" + those reporting that some of the food in question ,"X," they consumed was locally-produced

"Partial Subsistence" per-adult consumption =

$$\frac{\text{(Amount consumed of locally produced "X" by those only eating locally produced "X" and those eating both locally produced \& non-locally produced "X")}}{\text{(Those only eating locally produced "X" and those eating both locally \& non-locally produced "X")}}$$

3. "**Total Population**" = "Partial Subsistence" + those reporting that none of the food in question, "X," they consumed was locally produced.

"Total Population" per-adult consumption =

$$\frac{\text{(Amount consumed of locally produced X by those only eating locally produced "X" and those eating both locally produced \& non-locally produced "X")}}{\text{(Those only eating locally produced "X" \& those eating both locally \& non-locally produced "X" \& those not eating any locally produced "X")}}$$

Annual Adult Consumption Levels of Locally Produced Food and Tap Water Biosphere Study Area[1]
Table 6

Variable (Food Type)	"Total Population" Level[2] Sample n	Mean	Standard Deviation	"Partial Subsistence" Level[3] Sample n	Mean	Standard Deviation	"Subsistence" Level[4] Sample n	Mean	Standard Deviation
LeafyVeg.	1035	4.39	10.30	468	9.70	13.47	7	63.55	22.46
RootVeg.	1022	2.13	5.83	342	6.37	8.57	17	28.86	12.57
Grains	1021	0.40	4.37	37	11.01	19.24	1	60.64	18.82*
Fruit	1037	4.47	11.54	441	10.54	15.41	9	59.32	30.81
Poultry	1026	0.45	2.27	94	4.88	6.33	14	15.74	8.94
Meat	1025	0.92	4.97	109	8.66	13.04	63	8.97	10.07
Fish	1041	0.04	0.50	36	1.05	2.33	1	7.50	---**
Eggs	1021	2.32	5.51	327	7.28	7.79	93	15.78	7.58
Milk	996	4.84	19.94	80	60.50	49.59	28	119.39	26.27
TapWater[5]	1068	646.16	475.02	896	769.70	402.15	(896)	(769.70)	(402.15)

see notes on next page

Table 6 Notes

1. The study area is comprised of the following areas: Amargosa Valley, Beatty, Indian Springs, and Pahrump. All food amounts shown are in kilograms. Water and milk consumption are shown in liters. The summary statistics reflect weighting (post-stratification) by gender and area population and are provided for the resident adult population (18 years and over).

2. The denominators of the means of the "total population" consumption levels (per resident adult) INCLUDE all who responded to the question of whether or not they consumed locally-produced-food of the type in question. This denominator is comprised of those who report that: (a) nothing they consume is locally-produced; and (b) that "all," "some," or "very little" of the food type in question they consumed is locally-produced. Only those who responded "don't know" or refused to answer are excluded. Thus, the conceptual denominator is constant across all food types (including tap water): It is the total resident adult population of the Study Area.

3. The denominators of the means of the "partial subsistence" consumption levels (per resident adult) EXCLUDE those who report that nothing they consume is locally-produced. Those who responded "don't know" or refused to answer are also excluded. This denominator includes only those that report "all," "most," "some," and "very little," of the food type in question (that they consumed) is locally-produced. Thus, the conceptual denominator varies across food type and is comprised only of those adult residents who report consuming locally-produced food of the type in question.

4. The denominators of the means of the "subsistence" consumption levels (per resident adult) EXCLUDE those who report that either: (a) nothing they consume is locally-produced; or (b) that only "most," "some," or "very little," of the food type in question (that they consumed) is locally-produced. Those who responded "don't know" or refused to answer are also excluded. Thus, the conceptual denominator varies across food type and is comprised only of those adult residents who report that "all" of the food type in question they consumed is locally-produced.

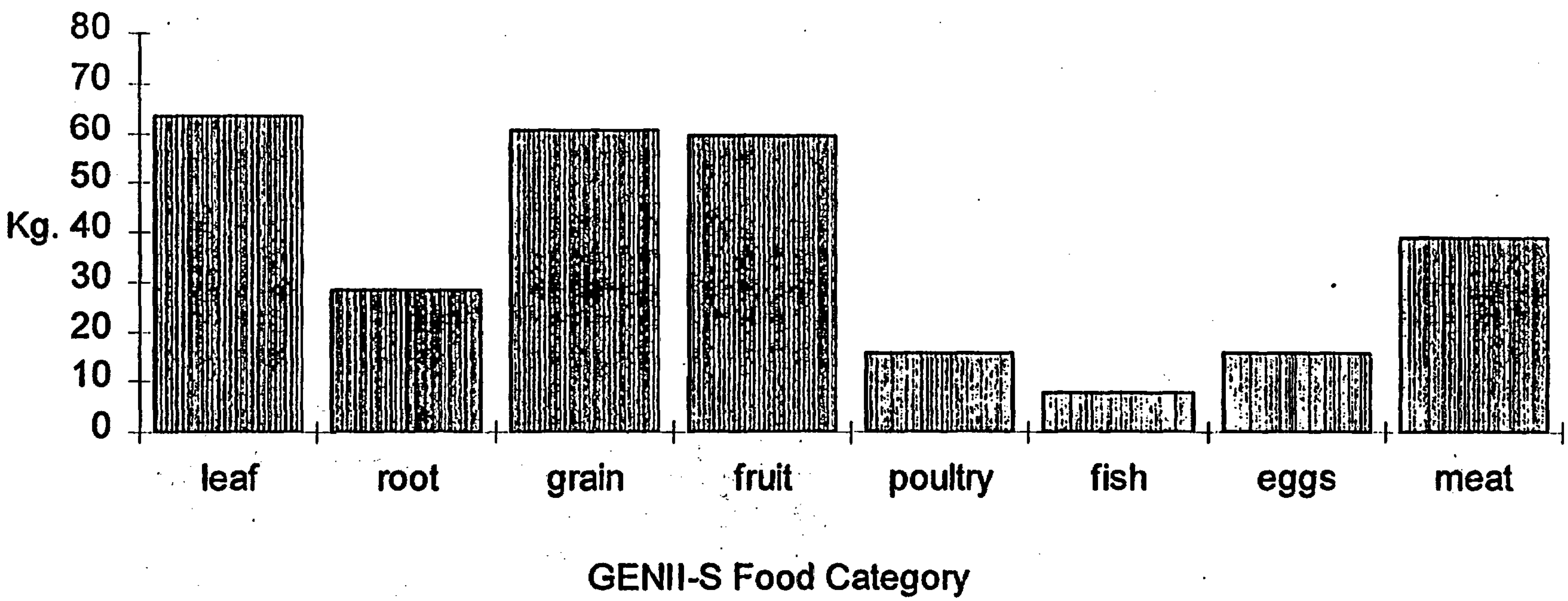
5. The denominator of the mean of the "total population" consumption level for tap water (per resident adult) INCLUDES those who responded as described in note 2 above. The denominator of the mean of the "partial subsistence" consumption level for tap water (per resident adult) EXCLUDES those reporting that they consume zero glasses of tap water per day. The water consumption question was asked in such a manner that precludes directly calculating a "subsistence" level. We assume that the "partial subsistence" mean approximates the subsistence mean.

* The standard deviation is calculated using weighted cases. There is actually more than one case but when summed the "weights" add up to approximately 1.00.

** Only one case was found for subsistence fish consumption.

Figure 1

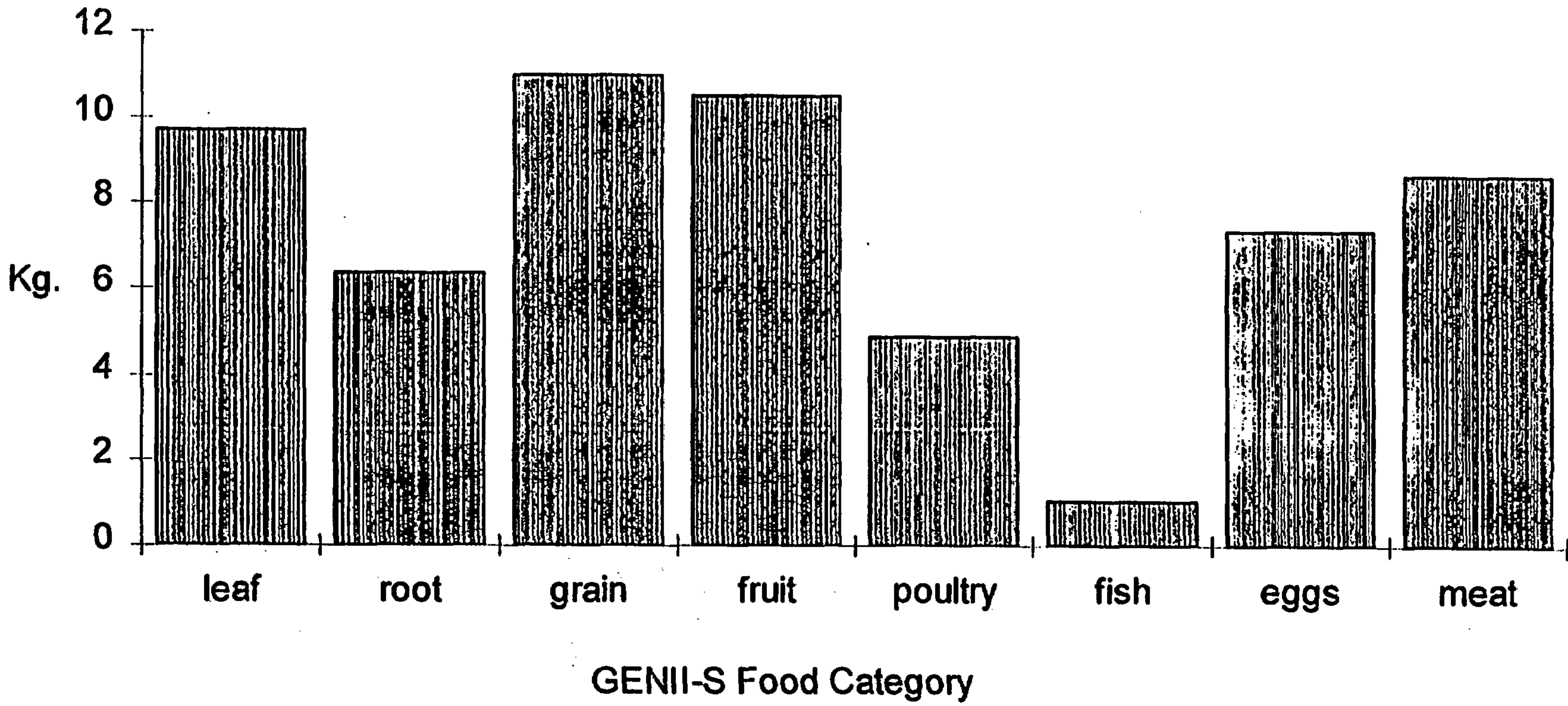
Annual "Subsistence" Per-Adult Consumption Level (kg.) of Locally Produced Food by GENII-S Food Category
Biosphere Study Area



Source: 1997 Biosphere Survey

Figure 2

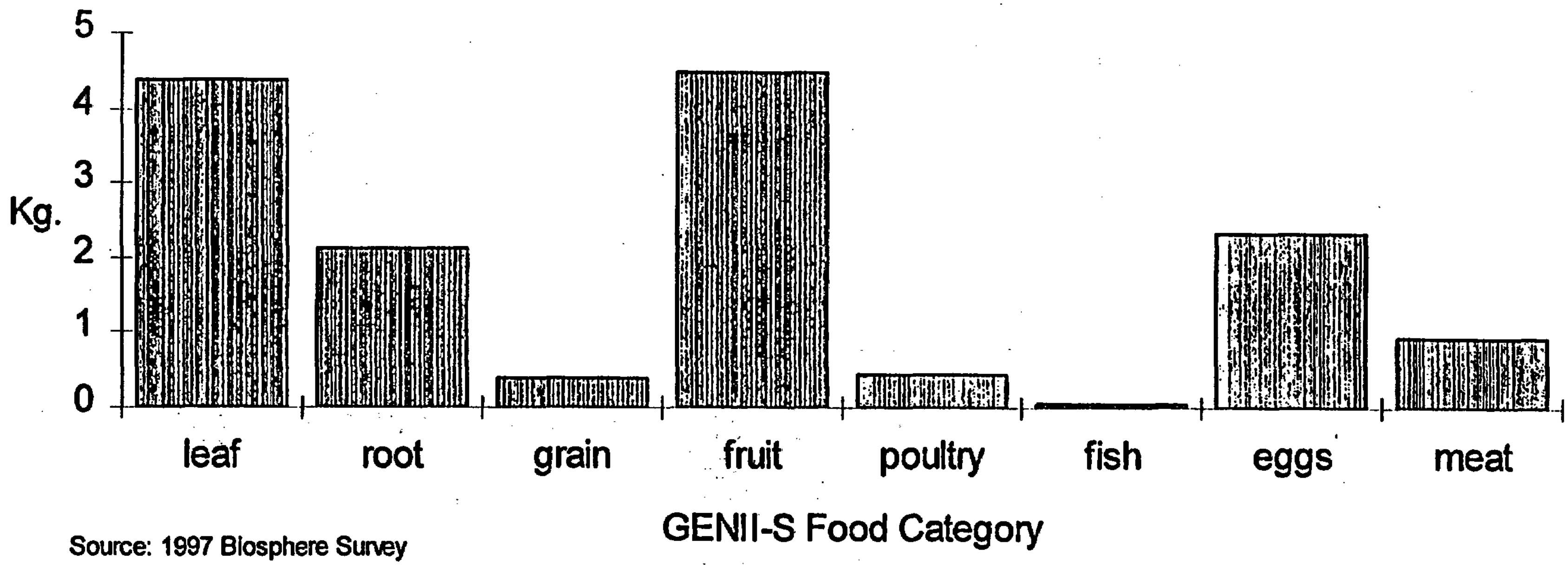
Annual "Partial Subsistence" Per-Adult Consumption Level (kg.) of Locally Produced Food by GENII-S Food Category Biosphere Study Area



Source: 1997 Biosphere Survey

Figure 3

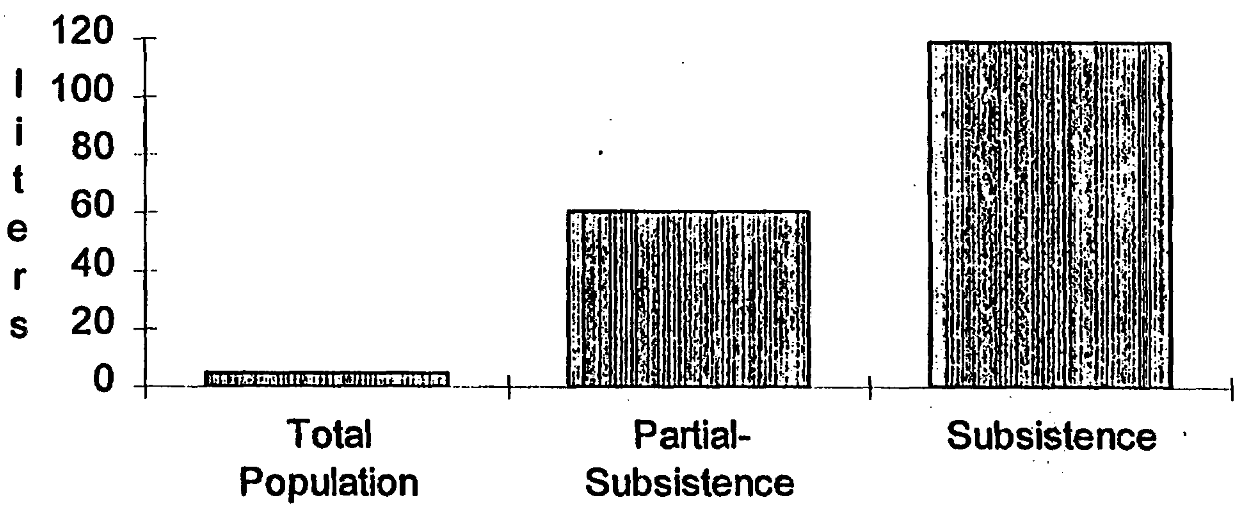
Annual "Total Population" Per-Adult Consumption level (kg.) of Locally-Produced Food by GENII-S Food Category Biosphere Study Area



Source: 1997 Biosphere Survey

Figure 4

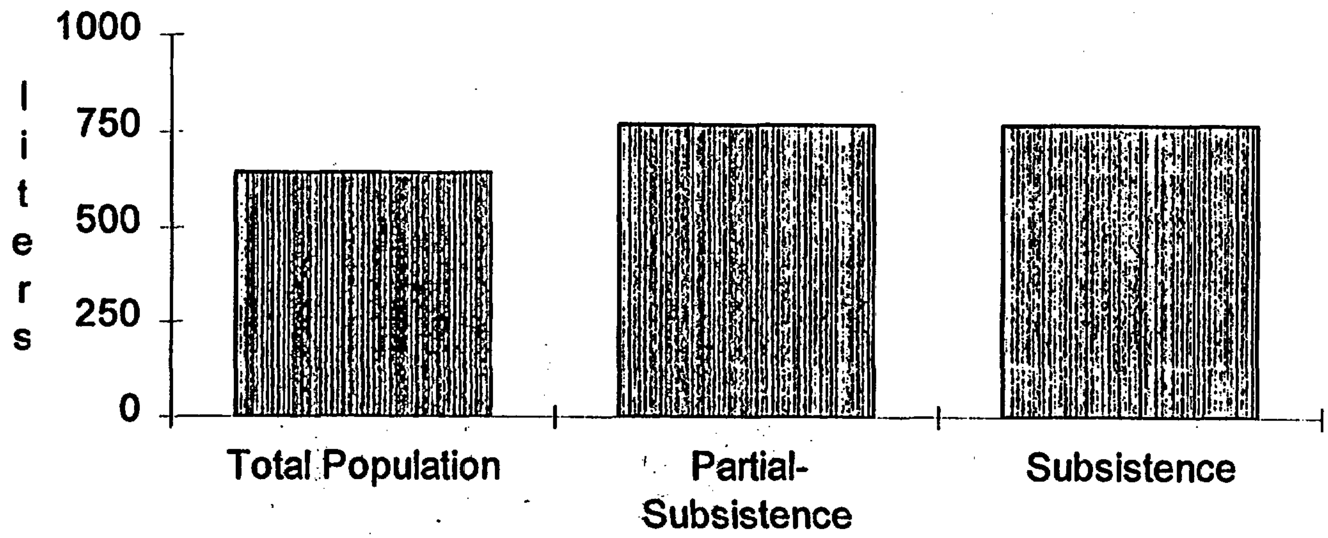
Annual Per-Adult Consumption of Locally Produced Milk: Total Population; Partial Subsistence; and Subsistence Biosphere Study Area



Source: 1997 Biosphere Survey

Figure 5

Annual Per-Adult Consumption of Tap Water: Total Population, Partial Subsistence, and Subsistence Biosphere Study Area

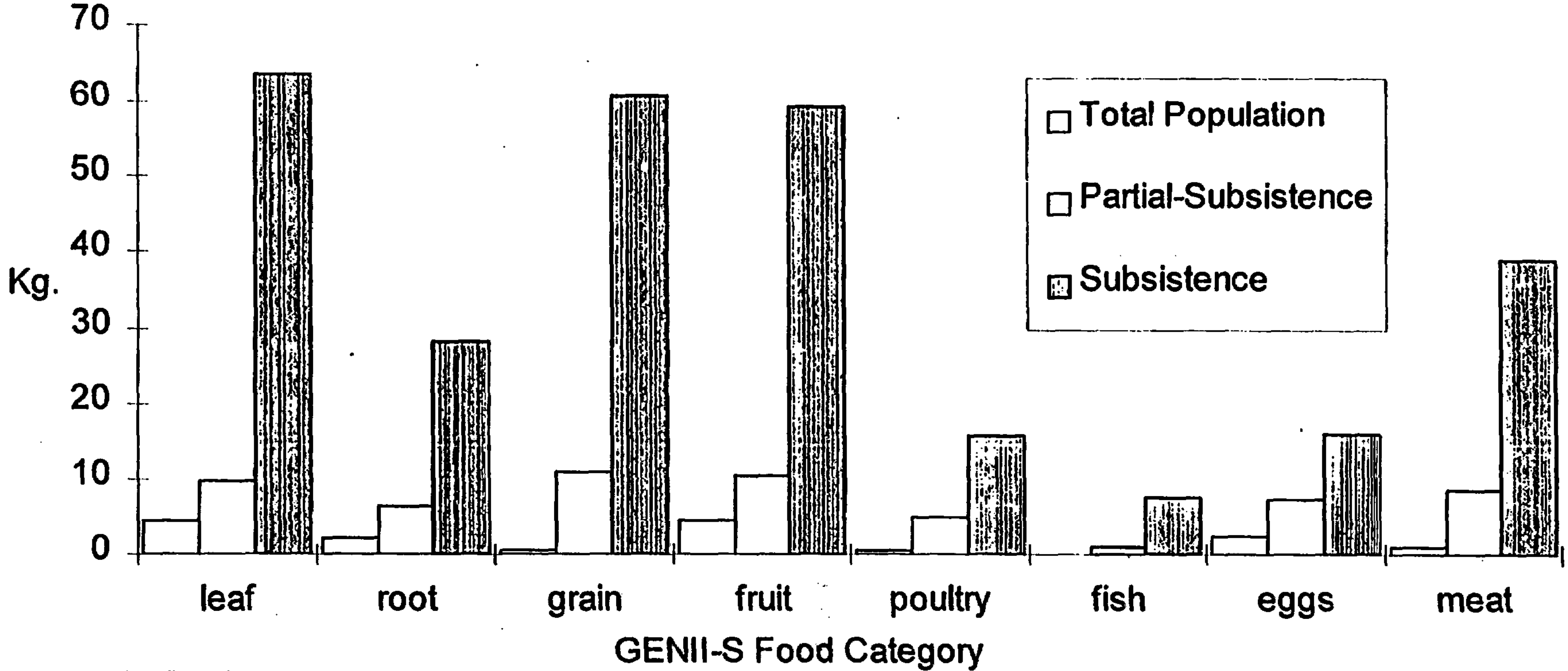


Source: 1997 Biosphere Survey

* The "subsistence" level is assumed to be equal to the "partial subsistence" level

Figure 6

Annual Per Adult Consumption of Locally Produced Food by GENII-S Food Group: Total Population, Partial Subsistence, and Subsistence Biosphere Study Area



Source: 1997 Biosphere Survey

Consumption Level Comparison
Table 7

Annual "Subsistence" Per-Adult Consumption Level of Locally-Produced Food (kg.) by Food Type and Milk/Water (Liter)

Dietary Data Resource	Fruits, Grains & Vegetables (Kg.)	Meat/ Poultry (Kg.)	Fish (Kg.)	Milk (liters)	Drinking Water (liters)
1997 Biosphere Subsistence[1]	211.8	54.7	7.7	119.4	769.7
1977 NRC Guide[2]	190	95	6.9	110	370
1994-95 USDA[3]	241.4	69.1	3.7	84.9	*
1974 USDA[4]	194	97.9	6.8	110.9	*

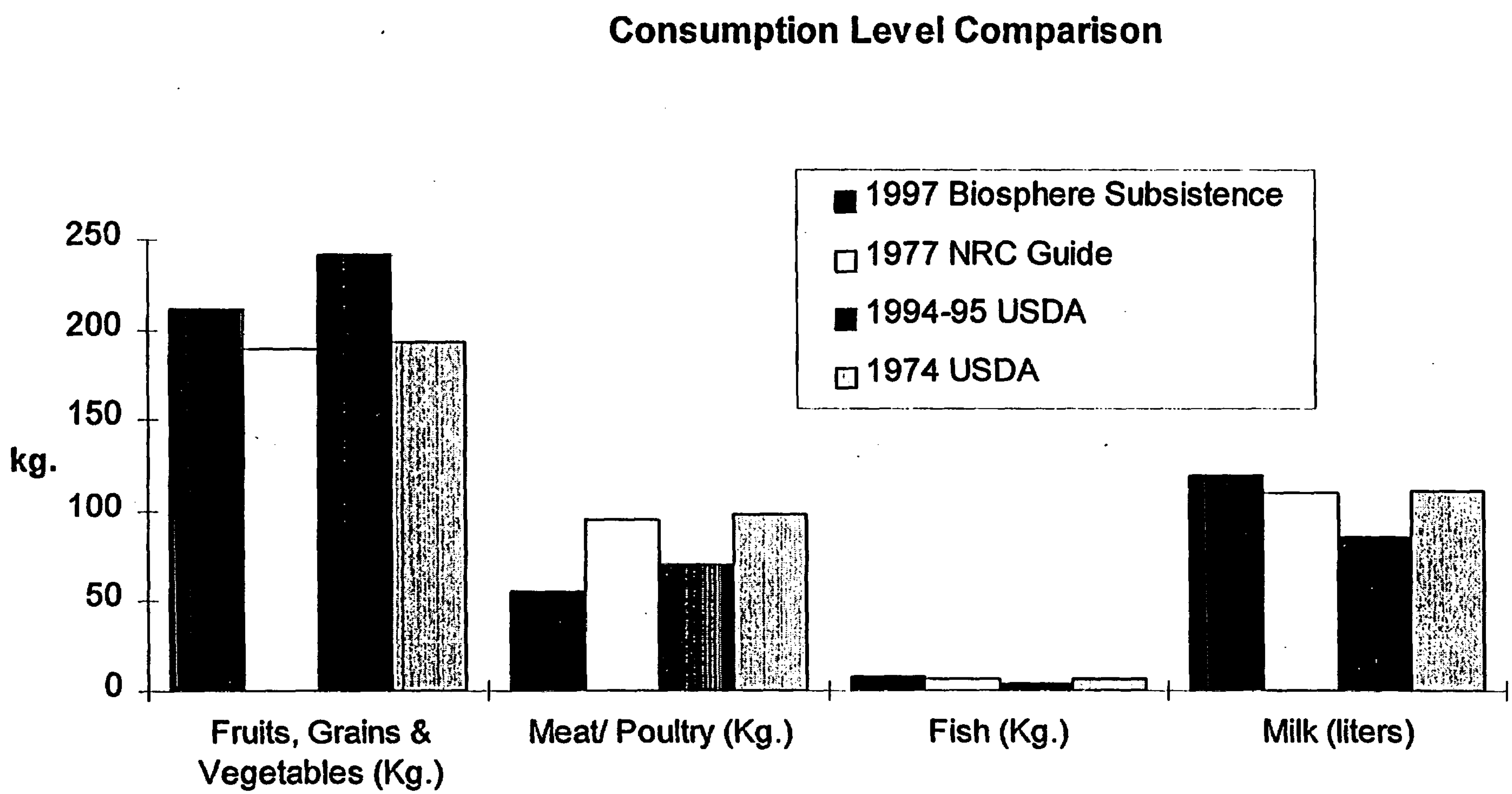
1 1997 Biosphere Survey. Data represent the "subsistence" consumption level

2 1977 NRC Guide.Table E-4, U.S. NRC Revision 1. Regulatory Guide 1.109. *"Calculation of Annual Doses to man from Routine Release of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR part 50, Appendix I." October, 1977*

3 1994-95 USDA. "*Data Tables: Combined Results From USDA's 1994 and 1995 Continuing Survey of Food Intake by Individuals for 1994 and 1995 Diet and Health Knowledge Survey*" Table 9 (http://www.barc.usda.gov/bhnrc/foodsurvey/home.htm) June, 1997.

4 1974 USDA. "Food Consumption, Prices and Expenditures" Supplement for 1974 to Agricultural Economic Report No. 138
Fruit, Grain and Vegetable values taken from Table 20
Milk caluclated by dividing lbs. of fluid milk equivalent by total, then applying ratio to calcium content basis, then multiplying by .95 (qts. to liters)
Fish taken from Table 6
Meat/Poultry taken from Table 6

Figure 7



Consumption Level Comparison
1997 Biosphere Subsistence
1977 NRC Guide
1994-95 USDA
1974 USDA
250
200
150
kg.
100
50
0
Fruits, Grains & Vegetables (Kg.)
Meat/ Poultry (Kg.)
Fish (Kg.)
Milk (liters)

Figure 8

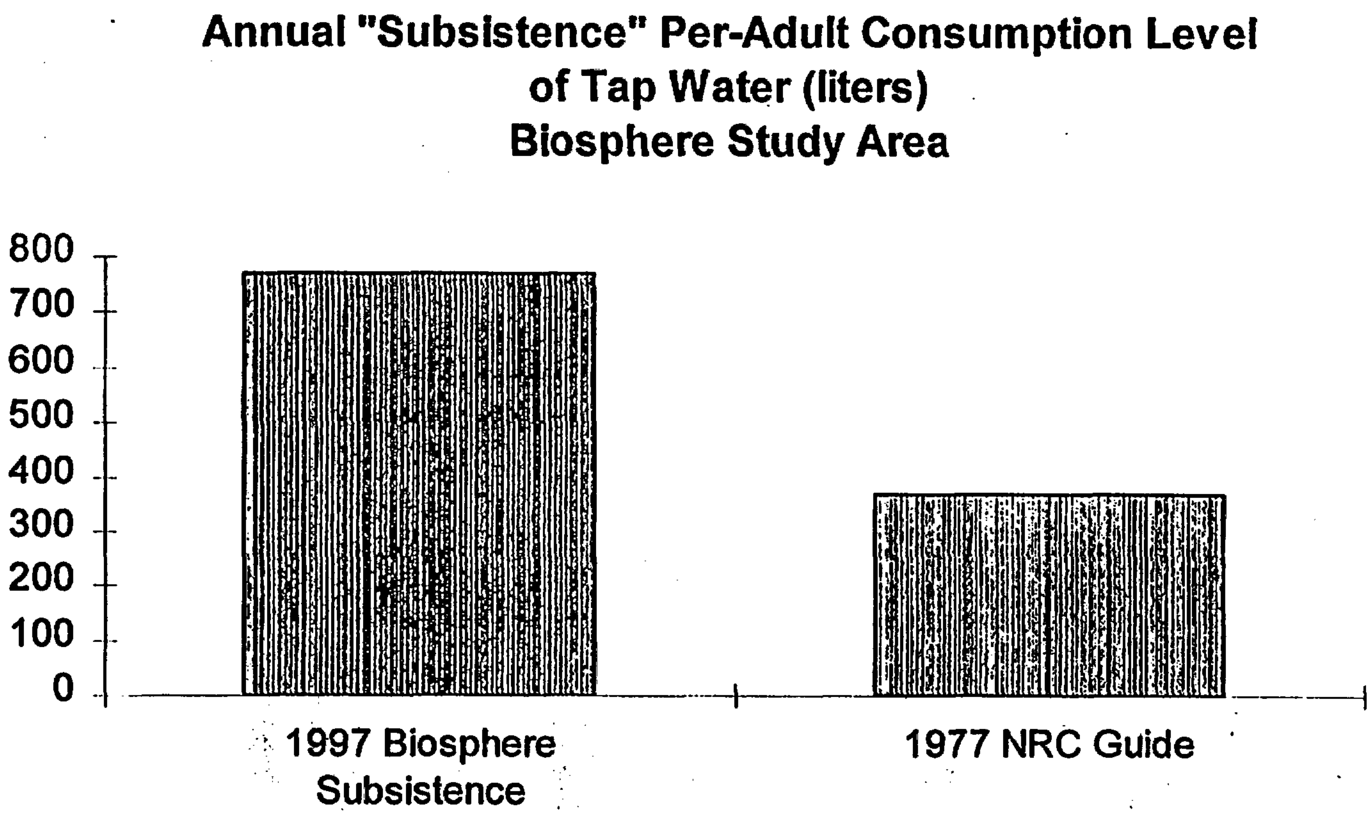
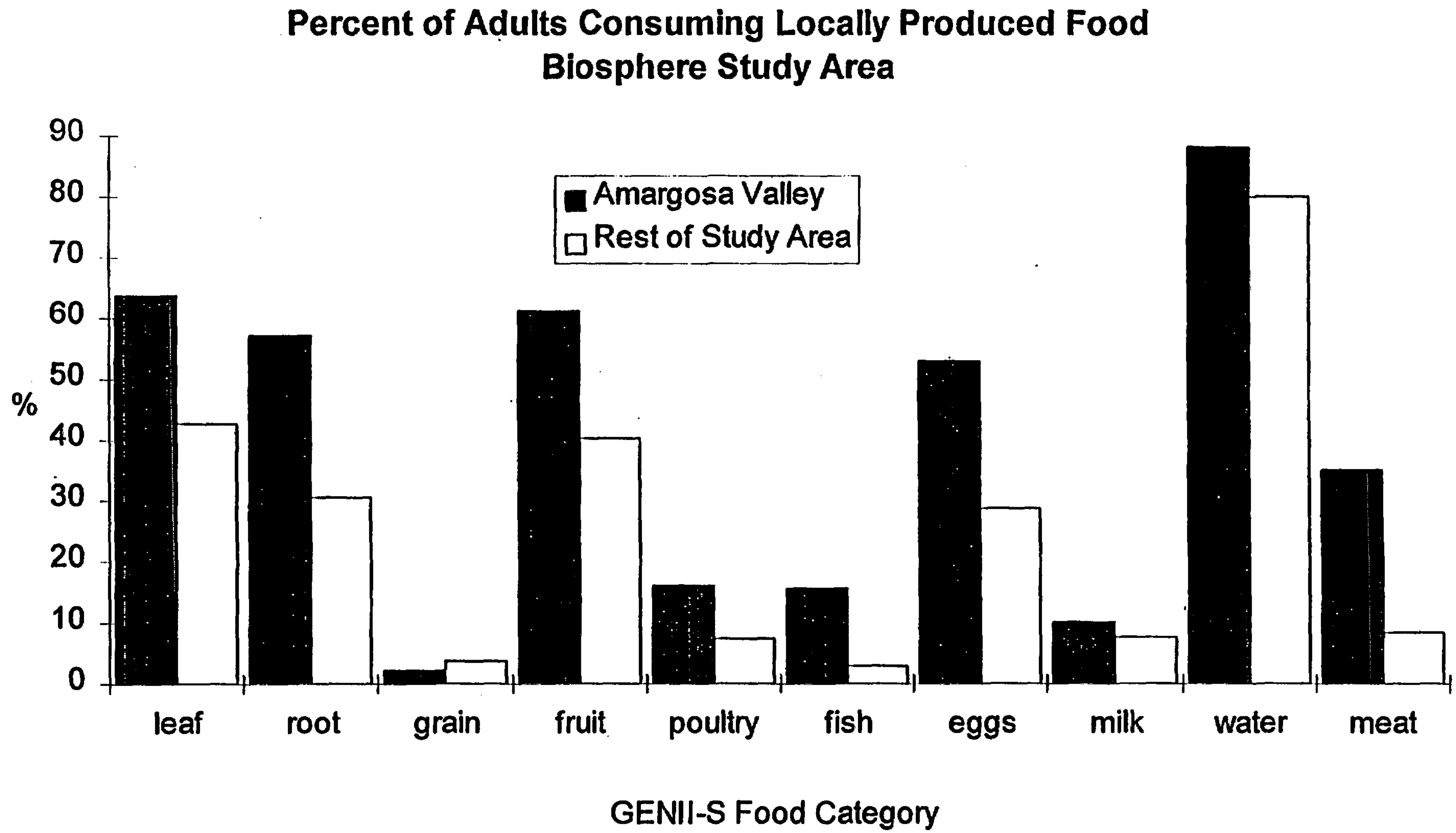

Annual "Subsistence" Per-Adult Consumption Level
of Tap Water (liters)
Biosphere Study Area
800
700
600
500
400
300
200
100
0
1997 Biosphere
Subsistence
1977 NRC Guide

Figure 9



Source: 1997 Biosphere Survey

Selected Socio-Economic Results (weighted)
Biosphere Study Area
Table 8

I. Household Characteristics*

Persons Per Household	2.58	
Housing Type	**Count**	**Percent**
single family house	389	36.15
trailer/mobile home	652	60.60
apartment	31	2.88
other	4	0.37
Household Income		
Under $25,000	283	31.88
With Garden	378	35.11
With Swamp Cooler	495	46.00
Total Households	**6,725**	**100.00**

II. Respondent Characteristics*

Respondent Age	**Count**	**Percent**
18-44 Years	364	34.31
45-64 Years	406	38.27
65 + Years	291	27.43
Respondent Race		
White	989	93.74
Amer. Indian	18	1.71
Black	7	0.66
Asian & Pac. Islander	6	0.57
Other	35	3.32
Hispanic Respondents	63	5.88
Total Adult Population	**12,876**	**100.00**

* Excluding the values shown for "Total Households" and "Total Adult Population," which are for the entire population, the denominator for each sample "percent" shown may vary slightly, depending upon the number responding. The correct sample percent denominator can be closely approximated by multiplying the value in the "count" column by 100 and then dividing this product by the corresponding value in the "percent" column. The absolute count for a given characteristic for the total households or the total adult population, respectively, can be approximated by using the "Total Household" and "Total Adult Population" values. For example, in the entire study area there are approximately 2,144 households with an income less than $25,000 ([6725*(31.88/100)] = 2,114) and 757 adults of Hispanic origin ([12876*(5.88/100)] = 757).

Selected Socio-Economic Results (weighted for gender)
Amargosa Valley
Table 9

I. Household Characteristics*

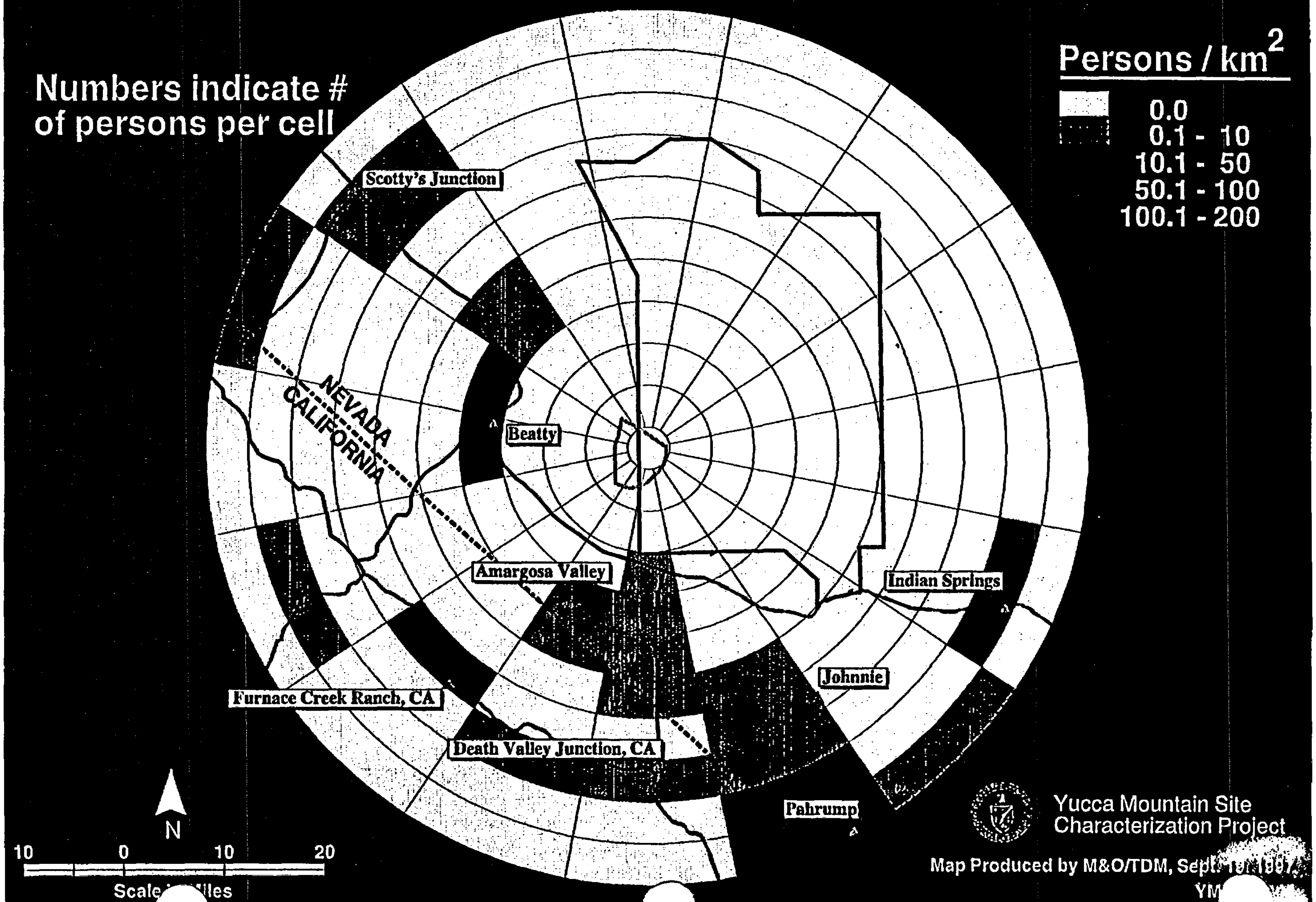
	Count	Percent
Persons Per Household	2.80	
Housing Type	**Count**	**Percent**
single family house	38	19.49
trailer/mobile home	154	78.97
apartment	2	1.03
other	1	0.51
Household Income		
Under $25,000	47	30.28
With Garden	89	45.72
With Swamp Cooler	142	72.80
Total Households	**452**	**100.00**

II. Respondent Characteristics*

Respondent Age	Count	Percent
18-44 Years	78	40.41
45-64 Years	79	40.93
65 + Years	36	18.66
Respondent Race		
White	172	88.66
Amer. Indian	2	1.03
Black	0	0.00
Asian & Pac. Islander	0	0.00
Other	20	10.31
Hispanic Respondents	24	12.27
Total Adult Population	**893**	**100.00**

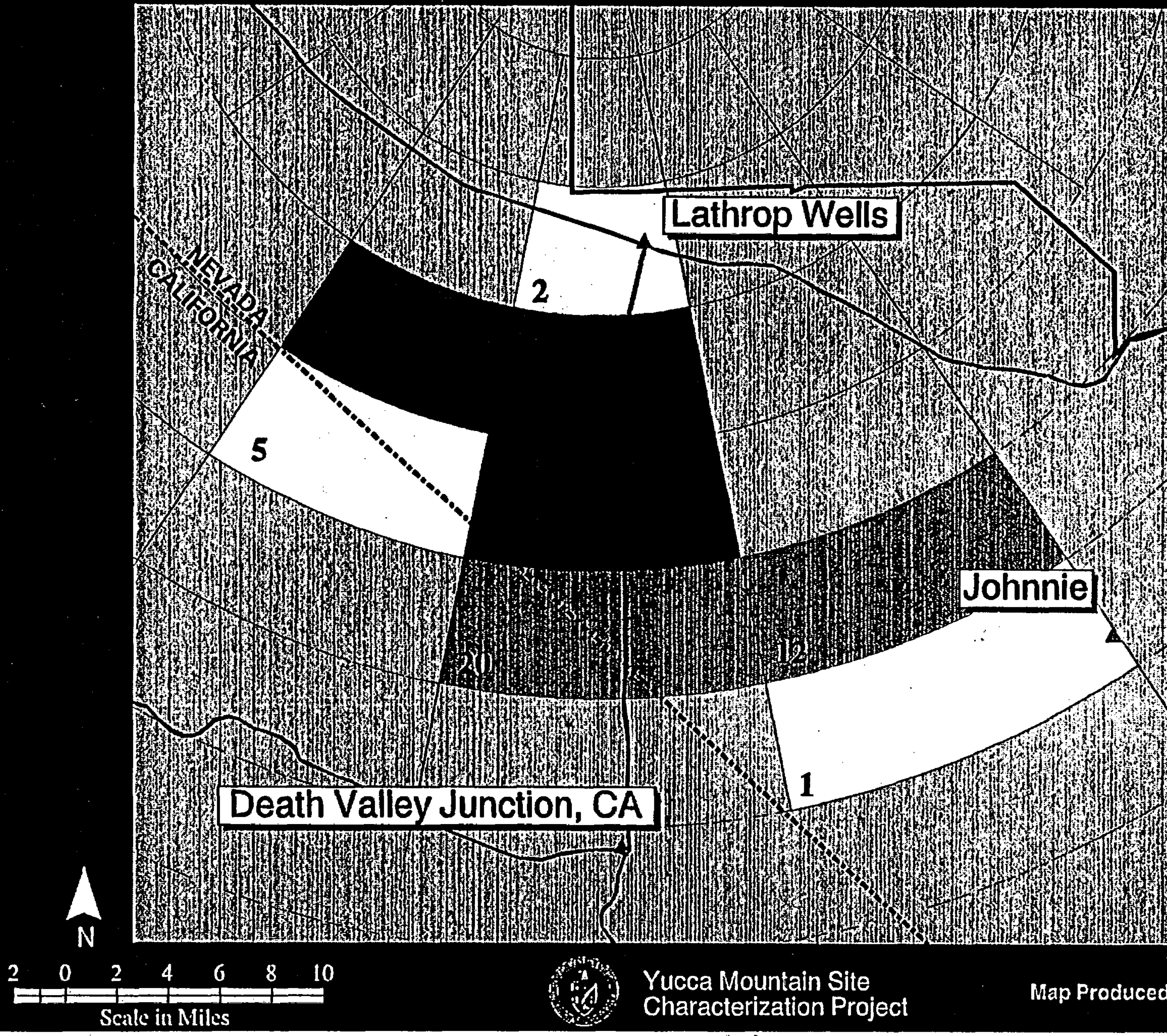
* Excluding the values shown for "Total Households" and "Total Adult Population," which are for the entire population, the denominator for each sample "percent" shown may vary slightly, depending upon the number responding. The correct sample percent denominator can be closely approximated by multiplying the value in the "count" column by 100 and then dividing this product by the corresponding value in the "percent" column. The absolute count for a given characteristic for total households or the total adult population, respectively, can be approximated by using the "Total Household" and "Total Adult Population" values. For example, in the Amargosa Valley, there are approximately 137 households with an income under $25,000 ([452*(30.28/100)] = 137) and 110 adults of Hispanic origin ([893*(12.27/100)] = 110).

EXHIBIT 1 - Population Density and Study Area



Map Produced by M&O/TDM, Sept.

EXHIBIT 2 - # of Interviews in Amargosa Valley



# of Interviews

- 0
- 01 - 05
- 06 - 10
- 11 - 30
- 30 - 100

Yucca Mountain Site Characterization Project

Map Produced by M&O/TDM, Sept. 19, 1997

YMP-97-268

V. Data Uses to-date and Current Developments

- Information from survey used to provide initial "Subsistence" food consumption input parameters for GENII-S, August 1997

- Information from survey used to provide alternative "total population" food consumption input parameters for GENII-S, September, 1997

- Information being analyzed for other EIS requirements, including Environmental Justice

- Lincoln County Survey (n=420) food consumption survey was completed in mid-October, data will be used in conjunction with "3X and 2X" (increased rainfall) climate change scenarios

VI. Discussion Issues

- If the protection standard is based on a critical group currently residing within the study area, we can provide its dietary and lifestyle characteristics using information from survey

- About 80 percent of the adults in the Amargosa Valley consume locally produced food and nearly 90 percent consume tap water

- Nowhere in the Amargosa Valley or elsewhere did the survey identify a respondent who reported that all of the food and water he or she consumed was locally produced

- The survey suggests that the Amargosa Valley is relatively homogenous with respect to diet and lifestyle

- GENII-S Sensitivity Runs

ATTACHMENT 21

YUCCA
MOUNTAIN
PROJECT

Studies

Yucca Mountain Biosphere Modeling

Presented to:

DOE/NRC Technical Exchange on Total System Performance Assessment

Presented by:

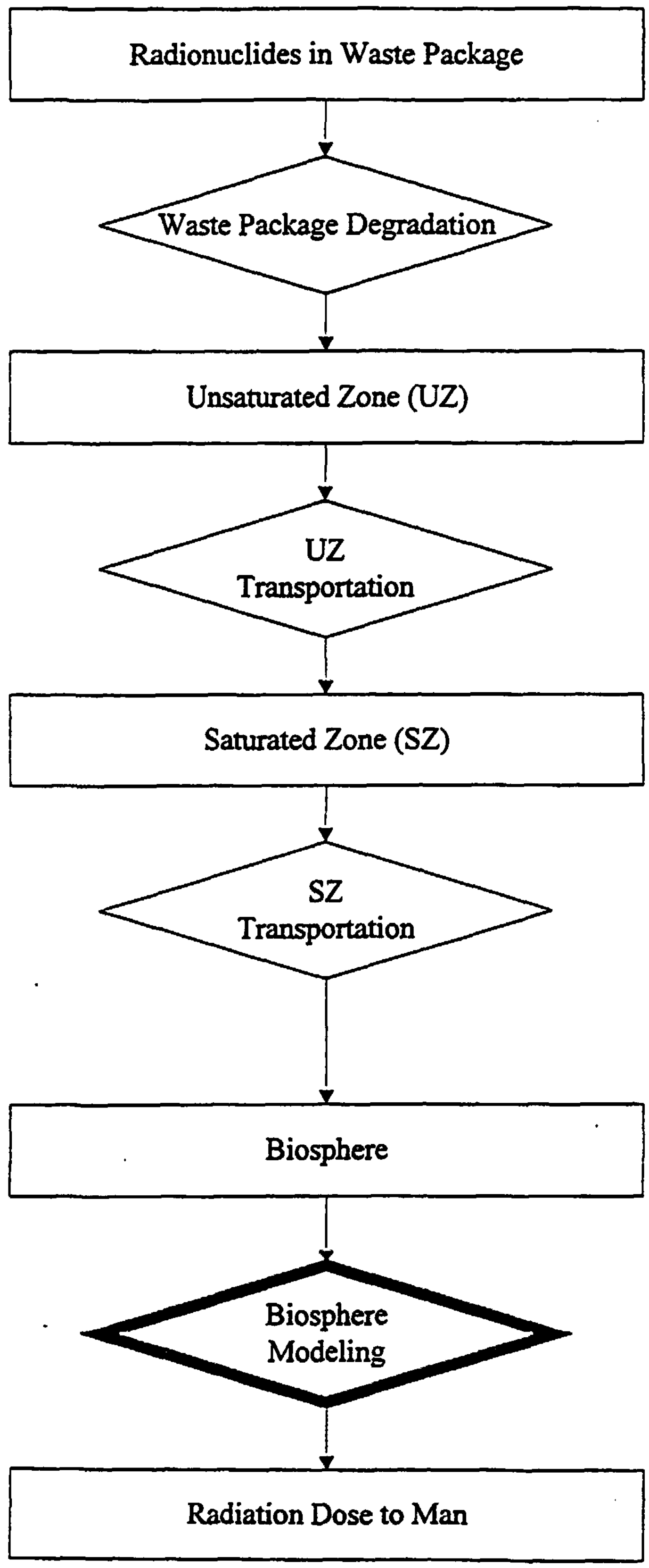
Jeffrey J. Tappen

Civilian Radioactive Waste Management System
Management and Operating Contractor
Las Vegas, Nevada

November 5, 1997

U.S. Department of Energy
Office of Civilian Radioactive
Waste Management

Biosphere Modeling in TSPA



J. Tappen/NRC/TEC-EX/11/05/97

Biosphere Definition

- The region of the earth in which environmental pathways for the transfer of radionuclides to living organisms are located and by which radionuclides in air, ground water, and soil can reach humans to be inhaled, ingested, or absorbed through the skin. Humans can also be exposed to direct irradiation from radionuclides in the environment (National Research Council, 1995).

Major Biosphere Modeling Assumptions

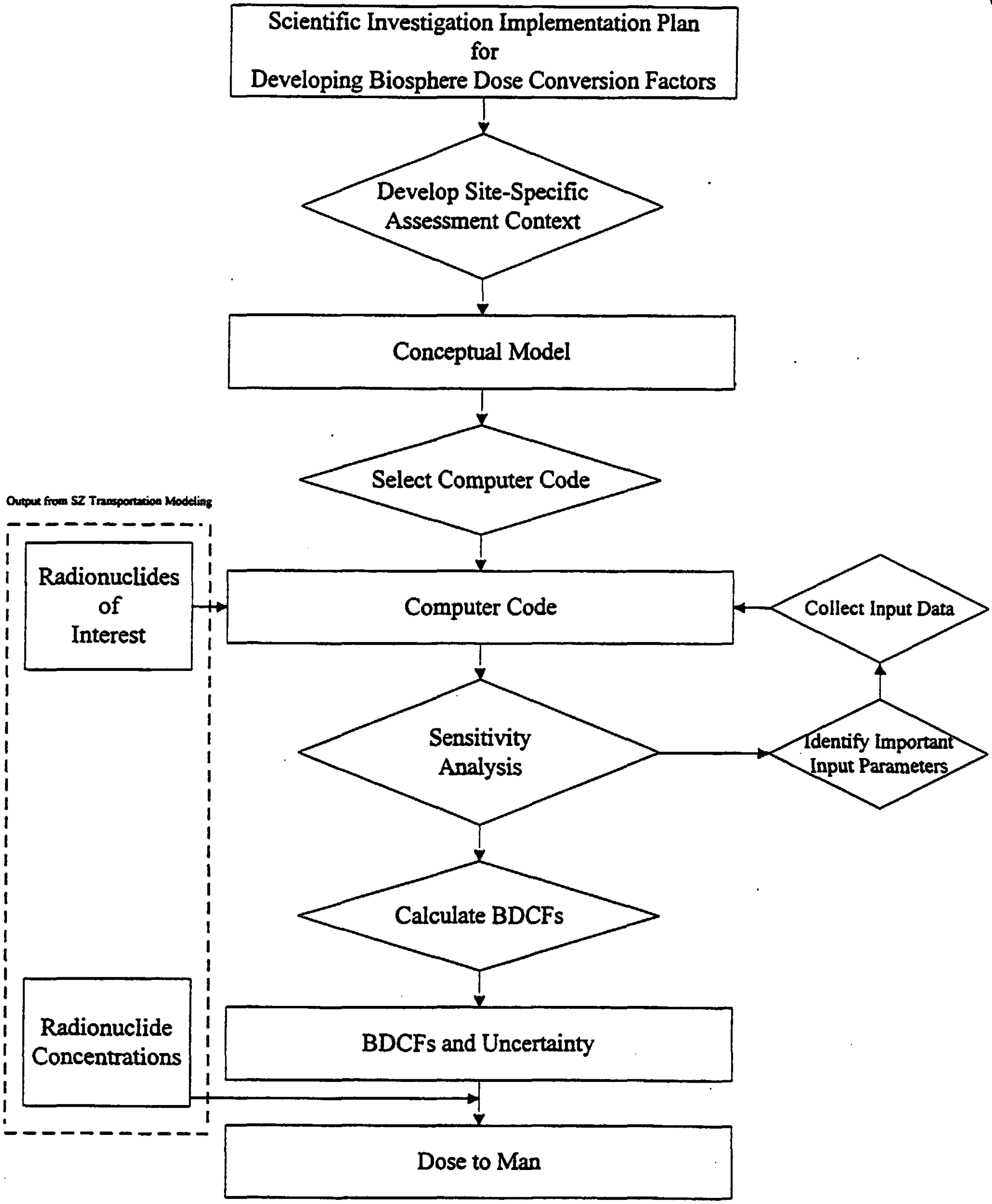
- Existing environmental conditions
- Use 20th century technology
- Adult / reference man

Biosphere Modeling Objectives

- Model radionuclide movement through the site-specific environmental pathways

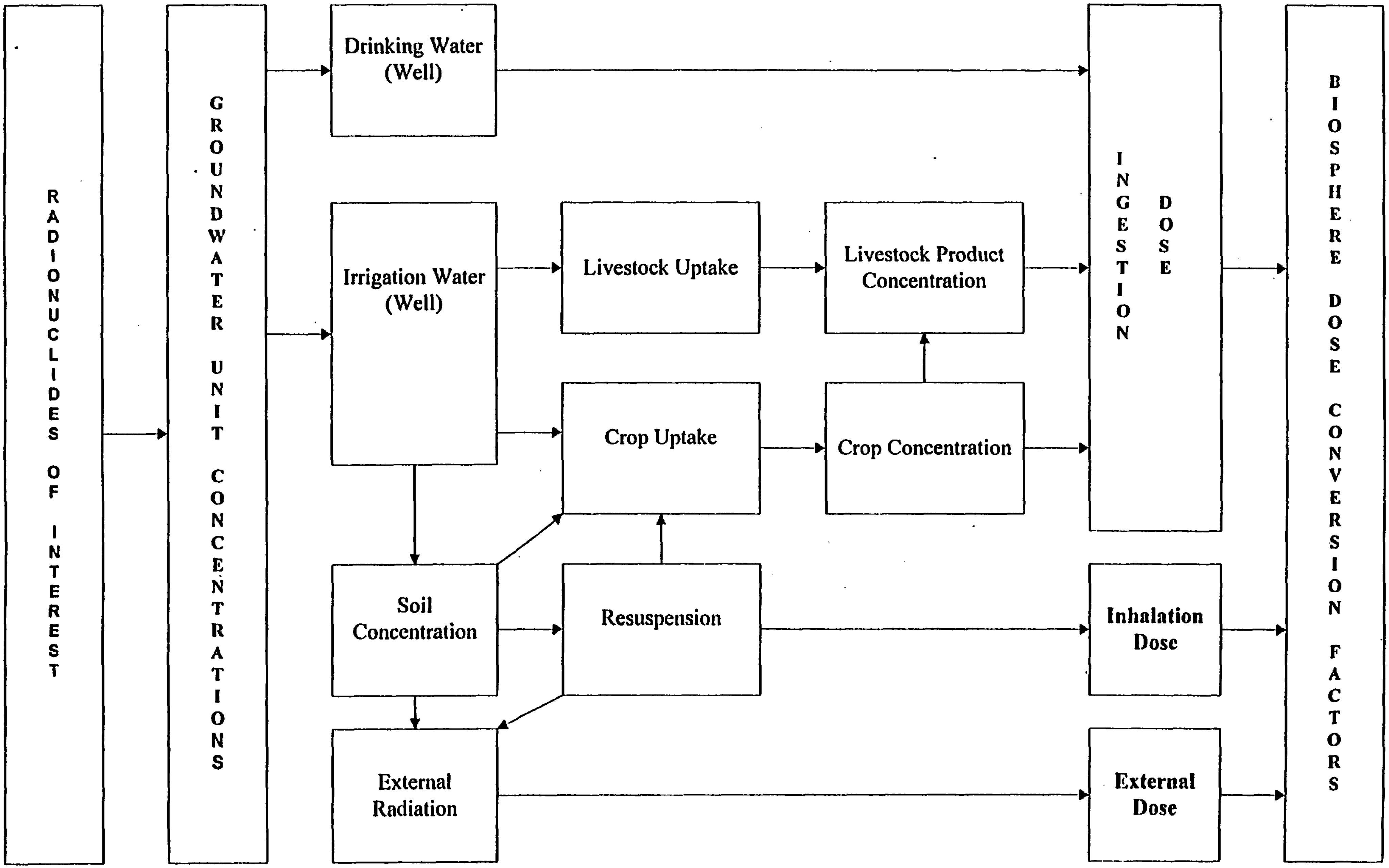
- Calculate Biosphere Dose Conversion Factors (BDCFs) for each radionuclide expected to enter the biosphere
  - Factor is the resulting Total Effective Dose Equivalent (TEDE) from unit radionuclide concentration in ground water, i.e., mrem/year/picoCurie/liter
  - Factors are scenario specific
    - Three receptors
      - Subsistence farmer, residential farmer, and average person in Amargosa Valley
    - Three precipitation states
      - 1X, 2X, and 3X

Biosphere Modeling



Development of Site-Specific Assessment Context and Conceptual Model

- Identify relevant site-specific features, events, and processes to be considered
  - environmental compartments
  - transport mechanisms
- Establish conceptual model



Human Exposure Pathways for Groundwater Release Scenario

J. Tappen/NRC…:C-EX/11/05/97

Evaluation and Selection of Computer Code

- Selection Criteria
  - existing, off-the-shelf
  - used in regulatory environment
  - capable of handling multiple scenarios
- Codes Evaluated
  - GENII-S, MEPAS, RESRAD, CAP88 PC, AIRDOS EPA, and RASCAL
- Code Selected: GENII-S

Data Collection and Sensitivity Analyses

- Use generic input data to perform sensitivity analyses
- Identify sensitive parameters and pathways
- Collect data with focus on sensitive parameters
- Repeat sensitivity analyses using collected data to confirm preliminary findings
- Finalize input parameters

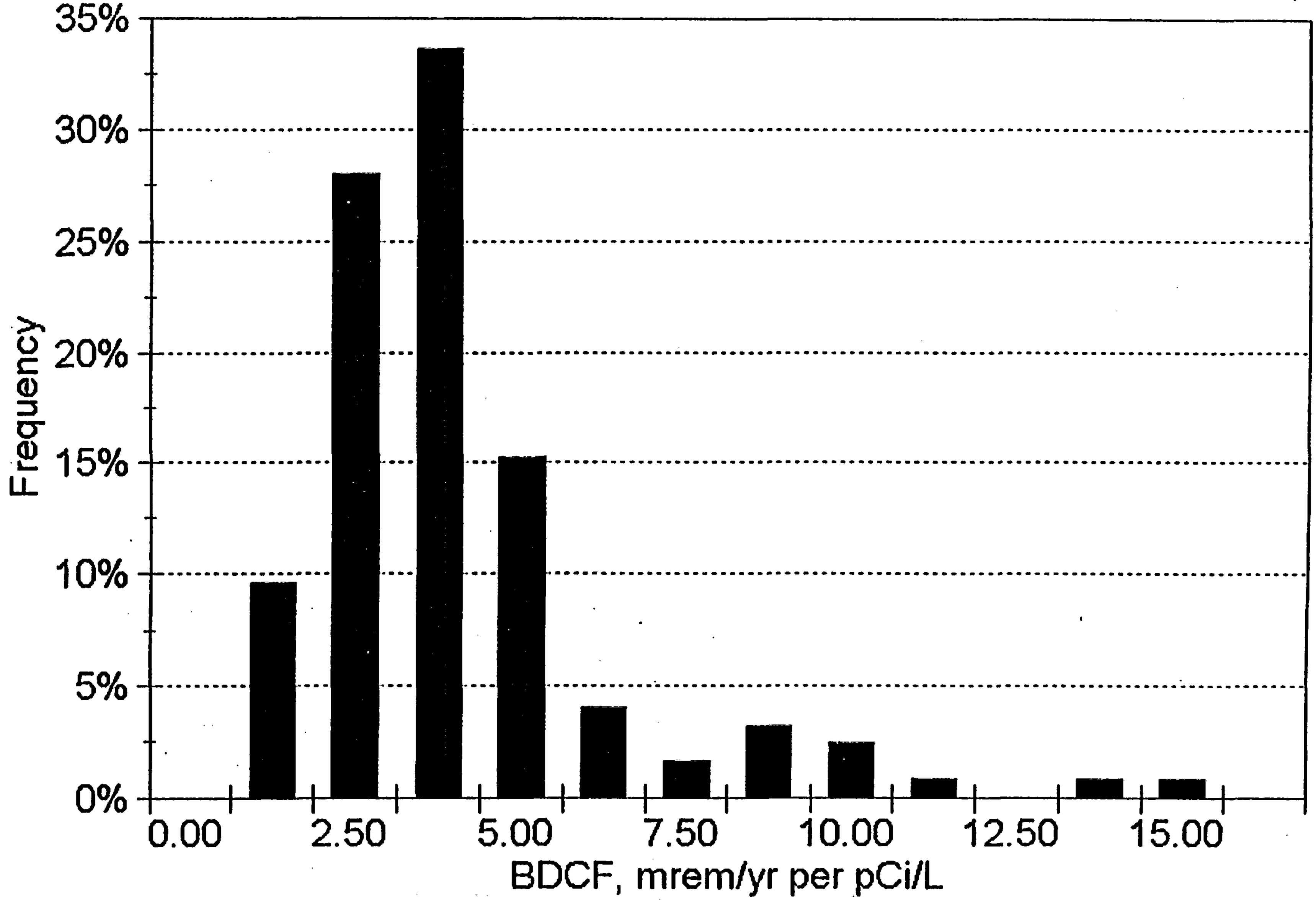
Site-Specific Data for Yucca Mountain

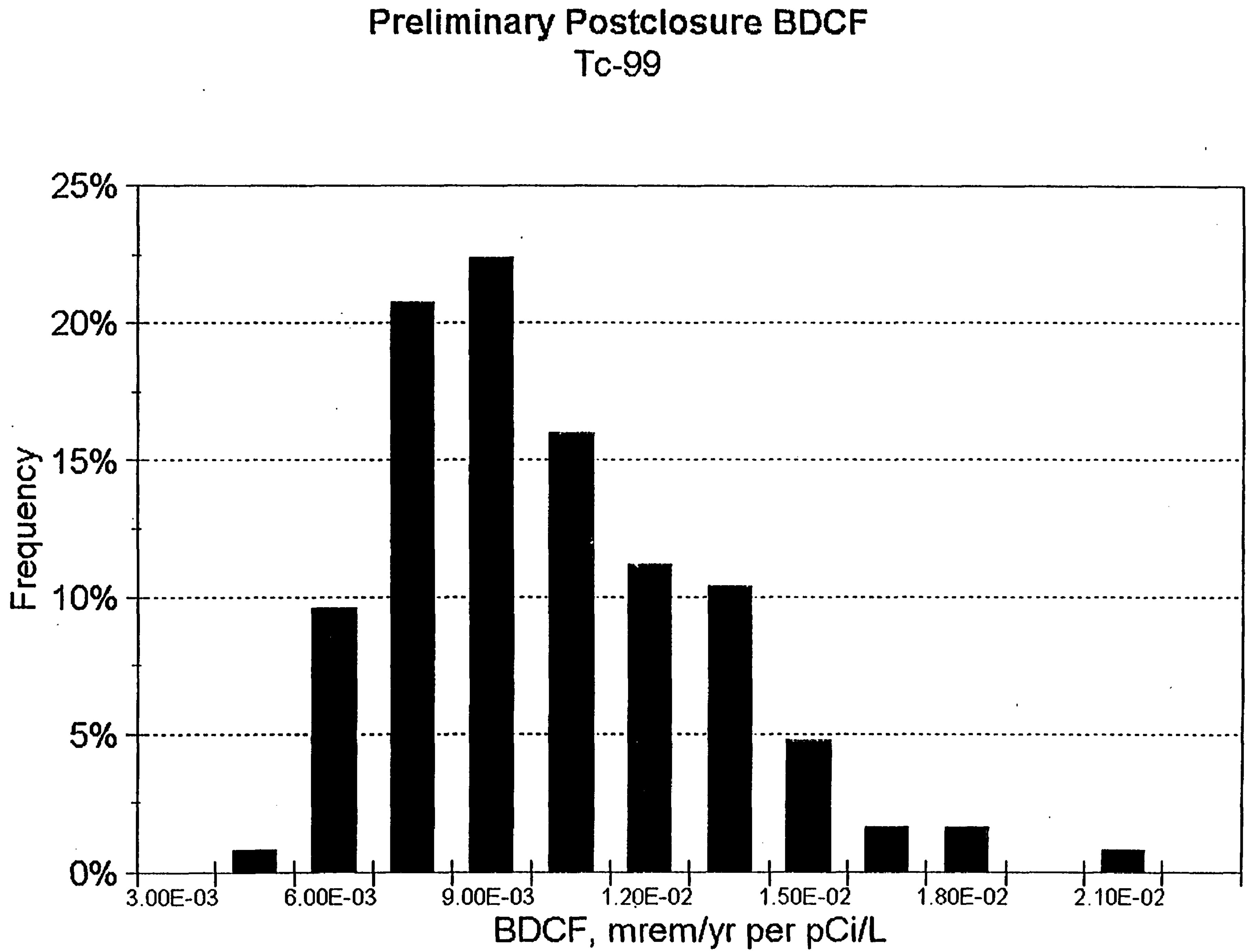
- Far field water monitoring
- Biotransport mechanisms and processes
- Soil types and characteristics
- Consumption of locally produced food

BDCF and Uncertainty

- Calculate BDCFs for
  - 39 radionuclides (TSPA/95)
  - 3 receptor scenarios
  - 3 precipitation states
- Evaluate uncertainties
  - sources
  - range

Preliminary Postclosure BDCF
I-129




Preliminary Postclosure BDCF
Tc-99
25%
20%
15%
10%
5%
0%
Frequency
3.00E-03
6.00E-03
9.00E-03
1.20E-02
1.50E-02
1.80E-02
2.10E-02
BDCF, mrem/yr per pCi/L

Biosphere Modeling Status

- Completed development of SIIP, site-specific assessment context, and selection of model
- Conducted initial sensitivity analyses
- Completed initial data collection and evaluation
- Deliver preliminary BDCFs - November 1997
- Update data collection and refine evaluation
- Deliver final BDCFs for TSPA/VA - March 1998

ATTACHMENT 22

NRC'S APPROACH TO SOURCE TERM MODELING

by

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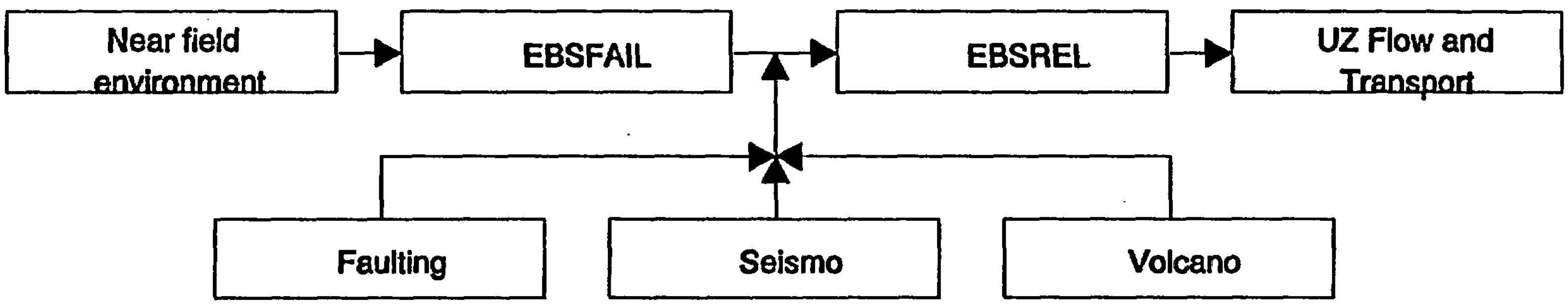
November 5-6, 1997
DOE/NRC Technical Exchange on
Total System Performance Assessments for Yucca Mountain

ENGINEERED BARRIER SYSTEM RELEASE (EBSREL) MODULE

- A consequence module of TPA Version 3.1 code



- A part of Engineering Barrier System Performance Assessment Code (EBSPAC) Version 1.1

- Calculates normalized radionuclide release rates from a subarea as a function of time

KEY ELEMENTS OF SUBSYSTEM ABSTRACTIONS

- Quantity and amount of water contacting waste forms
  - Dripping into drifts
  - Water entering waste containers
- Radionuclide release rates and solubility limits
  - Dissolution rates (increases with temperature)
  - Solubility limits (decrease with temperature for some radionuclides)
- Only spent fuel considered in the present model

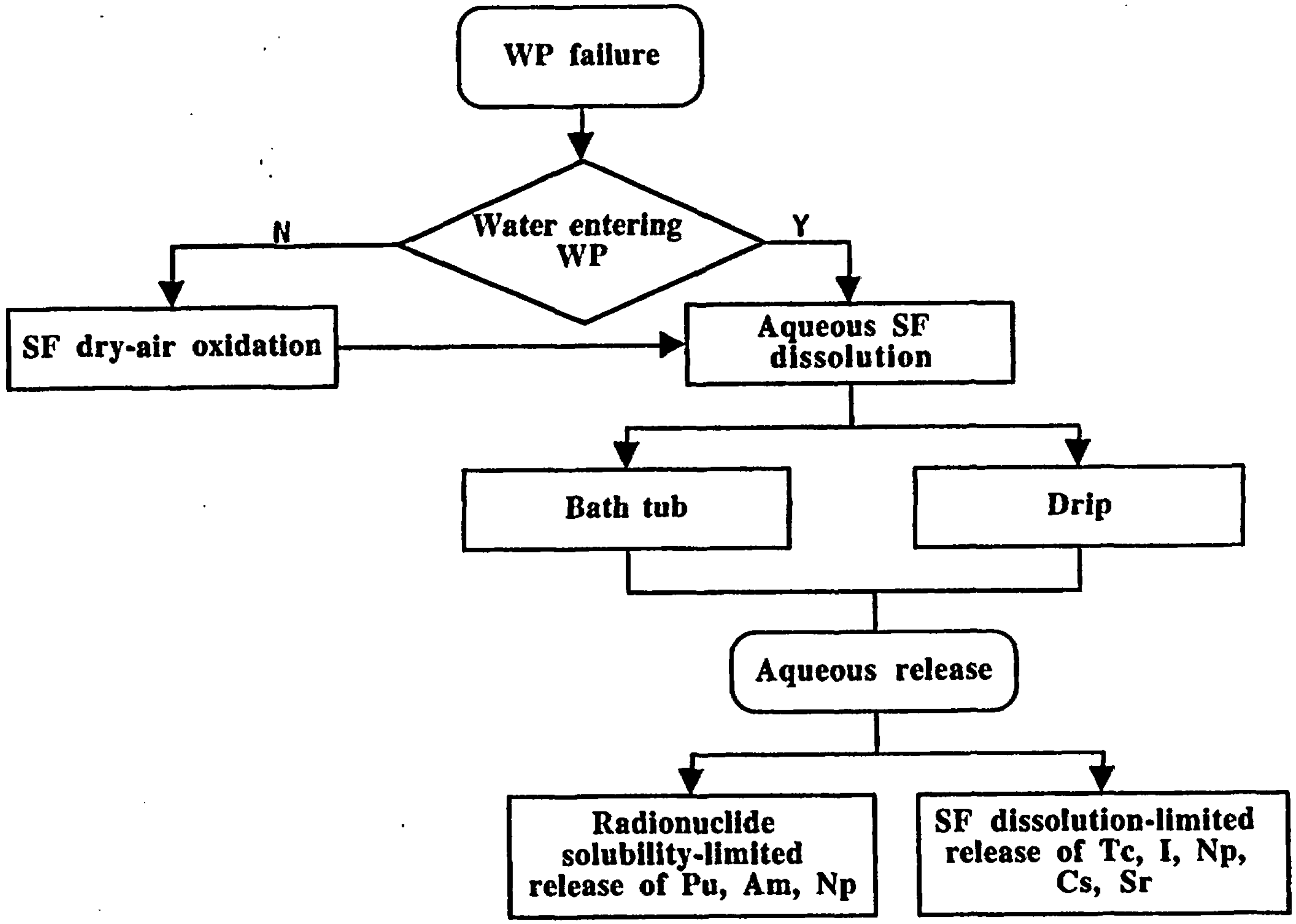
CONCEPTUAL MODEL APPROACHES

- Releases only from the wetted area of an SA
- Time-dependent water flow into the WP
- Advective and diffusive release from the EBS
- Waste form degradation
  - Waste forms dissolution rate; choice of SF dissolution models based on overall water chemistry: i.e., carbonate ion concentration, oxygen partial pressure, and pH, Ca and Si ions
  - Surface area exposed (with and without SF oxidation)
  - SF wetted fraction

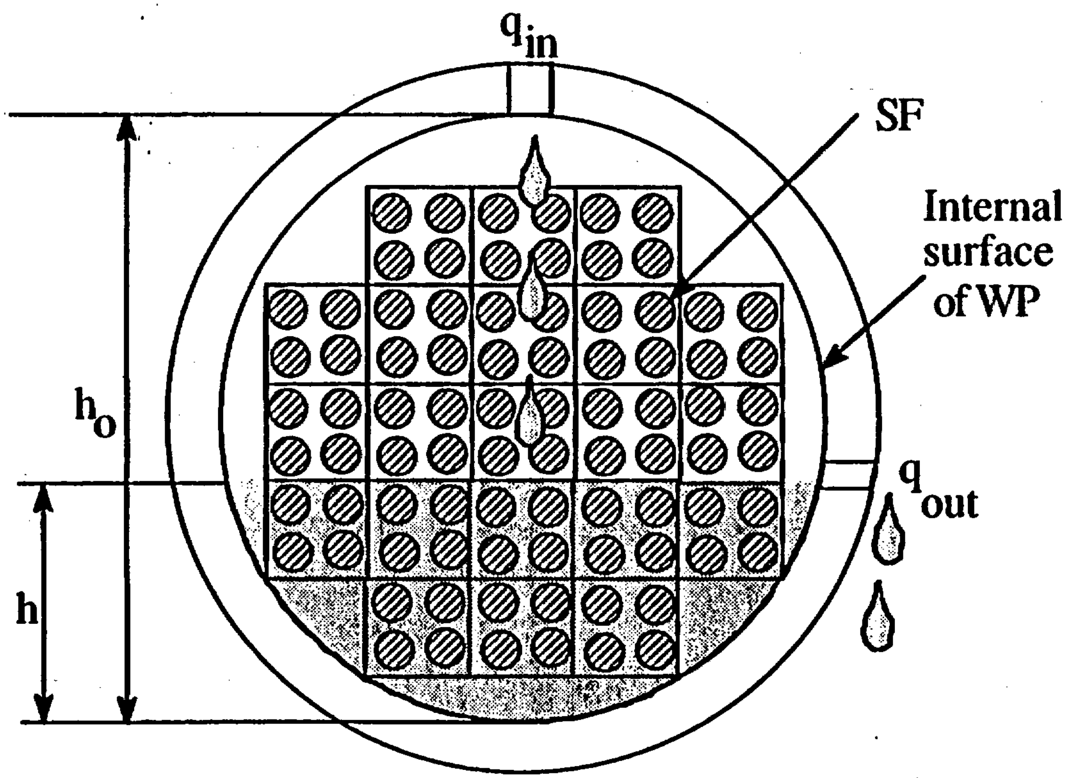
CONCEPTUAL MODEL APPROACHES (contd.)

- Radionuclide inventory: function of time due to ingrowth of daughter products
- Radionuclide release rates and solubility limits
  - Congruent dissolution of spent fuel
  - Dissolution rate versus solubility control
  - Different release models (bath tub, drip)
  - Flux through container
- Effect of cladding ignored but can be mimicked through data

RELEASE FROM EBS: FLOW DIAGRAM



BATHTUB MODEL FOR SPENT FUEL LEACHING



AQUEOUS RELEASE CALCULATIONS—ASSUMPTIONS

- All wetted and failed WPs in a subarea available for release simultaneously
- Release environment for a WP within a subarea is not affected by the presence of other neighboring WPs
- Backfill is considered to be present for diffusive release calculations
- At the time of failure, two holes (e.g., corrosion pits) are present on a WP: inlet and outlet port
- No new pits are formed that could alter the size of bath tub
- Flow in and out of the WP is independent of the size of these holes (i.e., no orifice effect); no barrier to flow due to corrosion products

AQUEOUS RELEASE CALCULATIONS—ASSUMPTIONS

- Water level cannot rise above the height of the outlet even at very large flow rates
- Liquid release takes place from the SF submerged in water; no liquid release from SF above water level
- Congruent release of RN (i.e., RN release to contacting water is proportional to the SF matrix leaching rate)
- RN not allowed to leave WP at a concentration higher than its solubility limit
- RN release occurs at a rate proportional to its mass fraction among all the isotopes of an element

UNCERTAINTIES IN RELEASE FROM EBS

- Amount of water contacting SF
- Radionuclide release rates and solubility limits
  - Rate controlling process (dissolution or solubility)
    - Solubility limits (Important for highly soluble radionuclides)
    - SF Leaching Parameters: Temperature, Oxygen partial pressure, Carbonate concentration, Wetted SF fraction, SF particle size , SF grain and sub-grain fragment size
  - Role of secondary minerals, cladding, and particle size

ATTACHMENT 23

TREATMENT OF BIOSPHERE ISSUES IN TPA 3.1 CODE

November 5-6, 1997
DOE/NRC Technical Exchange on
Total System Performance Assessments for Yucca Mountain

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Performance Assessment and HLW Integration Branch
Division of Waste Management

BACKGROUND

- IN ITS 1995 FINDINGS, THE NATIONAL ACADEMY OF SCIENCES (NAS) RECOMMENDED THAT DEVELOPMENT OF RISK-BASED STANDARDS FOR YUCCA MOUNTAIN STANDARDS USING THE "CRITICAL- GROUP APPROACH" BE USED
    - NAS CONCERNED ABOUT THE "EXTREME CASE DEFINED BY UNREASONABLE ASSUMPTIONS"
    - NAS RECOMMENDED USING "PRESENT KNOWLEDGE AND CAUTIOUS, BUT REASONABLE ASSUMPTIONS"
    - SUCH ASSUMPTIONS WOULD BE "LIFESTYLES, LOCATIONS, EATING HABITS, AND OTHER FACTORS"
- AS PART OF THE IMPLEMENTATION OF ITS ITERATIVE PERFORMANCE ASSESSMENT (IPA) CAPABILITY, THE NRC STAFF HAS BEEN EVALUATING THE NAS FINDINGS AND RECOMMENDATIONS
    - STAFF INTERESTED IN UNDERSTANDING HOW DOSE ESTIMATES VARY OVER TIME AND SPACE IN THE NTS/YUCCA MOUNTAIN AREA
    - *DILUTION* AND *LIFESTYLE* ARE ANTICIPATED TO HAVE AN IMPORTANT INFLUENCE ON DOSE

TODAY'S PRESENTATIONS

- DILUTION —
  - SCOPING STUDY OF DISPERSION IN THE SATURATED ZONE:
    BOB BACA et al./CNWRA
  - USE OF GROUND WATER IN THE ARID AND SEMI-ARID WESTERN UNITED STATES:
    GORDON WITTMEYER et al./CNWRA
- LIFESTYLES —
  - DOSE CONVERSION FACTORS IN TPA VERSION 3.1 COMPUTER CODE:
    PAT LAPLANTE/CNWRA
- **THE APPROACHES AND ASSUMPTIONS USED IN TPA 3.1 CODE SHOULD IN NO WAY BE CONSTRUED TO EXPRESS THE VIEWS OR PREFERENCES OF THE STAFF ON WHAT THE NATURE OF A FUTURE NRC IMPLEMENTING RULE SHOULD BE**

ATTACHMENT 24

SCOPING STUDY OF DISPERSION IN THE SATURATED ZONE

by

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November 5-6, 1997
DOE/NRC Technical Exchange on
Total System Performance Assessment for Yucca Mountain

PRESENTATION OUTLINE

- Objectives of Scoping Study
- Modeling Approach
- Data and Major Assumptions
- Simulation Results
- Summary

OBJECTIVES OF SCOPING STUDY

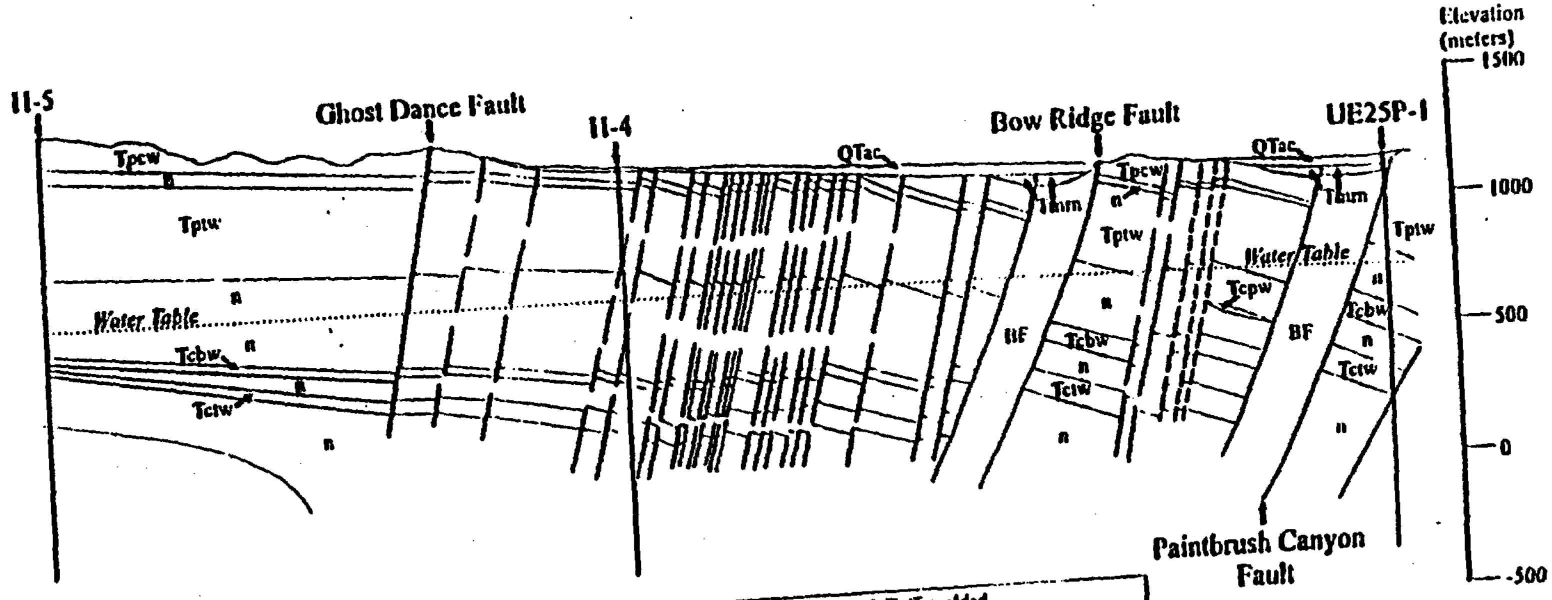
- Gain insight into site specific factors that may affect groundwater mixing and attendant dilution of dissolved radionuclides at the YM site
  - geometry of hydrostratigraphic units
  - contrasts in saturated hydraulic conductivity
  - variability of effective porosity
  - variability of mass dispersivities
  - location and properties of fault zones
- Develop better estimates of dilution factors using detailed models and available geologic and hydrologic data

MODELING APPROACH

- Conduct a set of 2D computer simulations* of groundwater flow and transport. Compute four quantities to relate dilution to flow characteristics:
  - hydraulic head distributions
  - groundwater flow paths
  - particle travel times and isopleths
  - plume distributions

* NRC High-Level Radioactive Waste Program Annual Progress Report: FY 1996 (NUREG/CR-6513)

Geologic Cross-section



Tpcw	Tiva Canyon Member of Paintbrush Tuff, welded
n	Nonwelded tuff
Tptw	Topopah Spring Member of Paintbrush Tuff, welded
Tcbw	Bullfrog Member, welded
Tctw	Tram Member, welded
QTac	Alluvium and Colluvium
BF	Zone of west-dipping strata containing abundant breccia and faults
Tmm	Rainier Mesa Member of Timber Mountain Tuff, nonwelded
Tcpw	Prow Pass Member of Crater Flat Tuff, welded

Source: Scott and Bonk, USGS OFR 84-494 (1984).

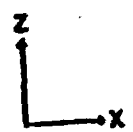
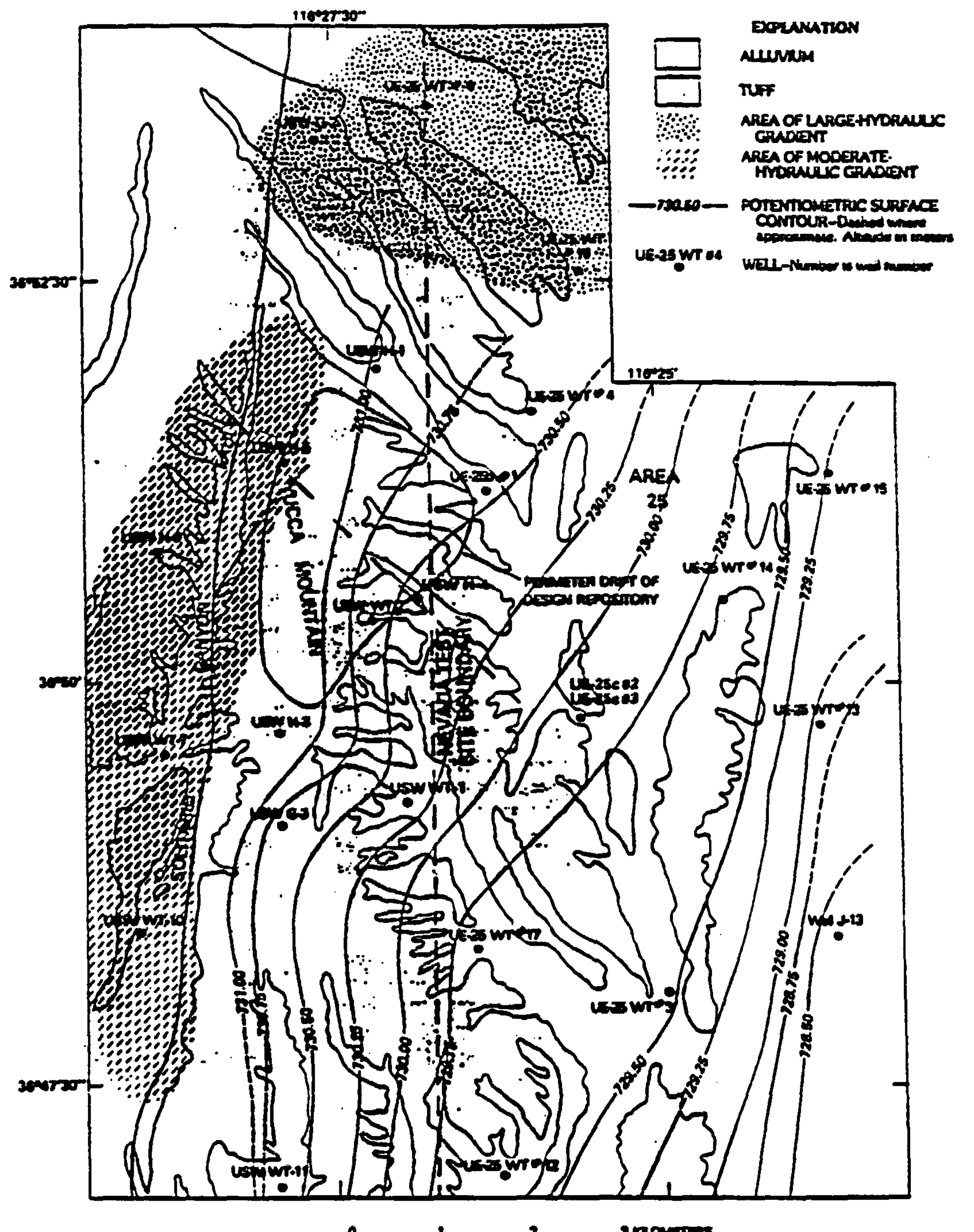
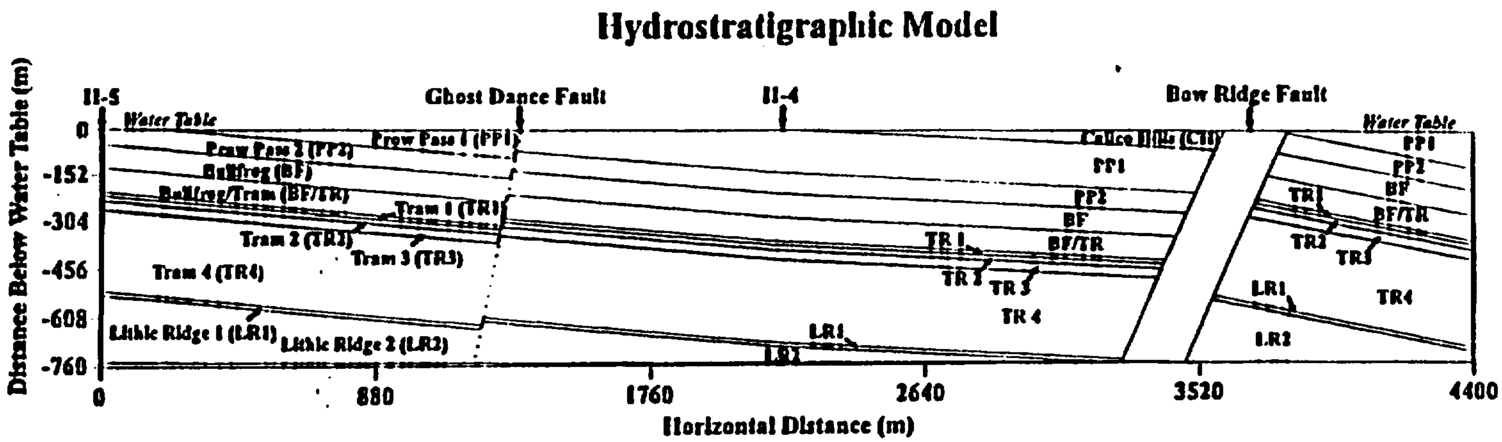


Figure 2-2. Vertical cross section through boreholes USW H-5 and USW H-4 (Scott and Bonk, 1984)


EXPLANATION
ALLUVIUM
TUFF
AREA OF LARGE-HYDRAULIC GRADIENT
AREA OF MODERATE-HYDRAULIC GRADIENT
730.50 POTENTIOMETRIC SURFACE CONTOUR—Dashed where approximate. Altitude in meters
UE-25 WT #4 WELL—Number is well number
116°27'30"
116°25'
36°52'30"
36°50'
36°47'30"
YUCCA MOUNTAIN
NEVADA TEST SITE BOUNDARY
AREA 25
PERIMETER DRIFT OF DESIGN REPOSITORY
UE-25 WT #4
UE-25 WT #15
UE-25 WT #14
UE-25c #2
UE-25c #3
UE-25 WT #13
USW WT-1
USW G-3
USW H-3
UE-25 WT #17
Well J-13
UE-25 WT #3
USW WT-11
UE-25 WT #12
731.00
730.75
730.50
730.25
730.00
729.75
729.50
729.25
729.00
728.75
728.50
0 1 2 3 KILOMETERS
0 1 MILE

DATA AND MAJOR ASSUMPTIONS

- Isothermal steady flow
- Hydraulic gradient of 3×10^{-3} (Calibration of 2D planar flow model)
- Hydraulic conductivities from borehole H-4 (Whitfield et al., 1985)
- Effective porosities $0.003 \leq \phi \leq 0.07$ (inferred from specific yield data)
- Dispersivities $\alpha_L = 30$ m & $\alpha_T = \alpha_L/10 = 3$ m
- Nonsorbing radionuclide with long half-life



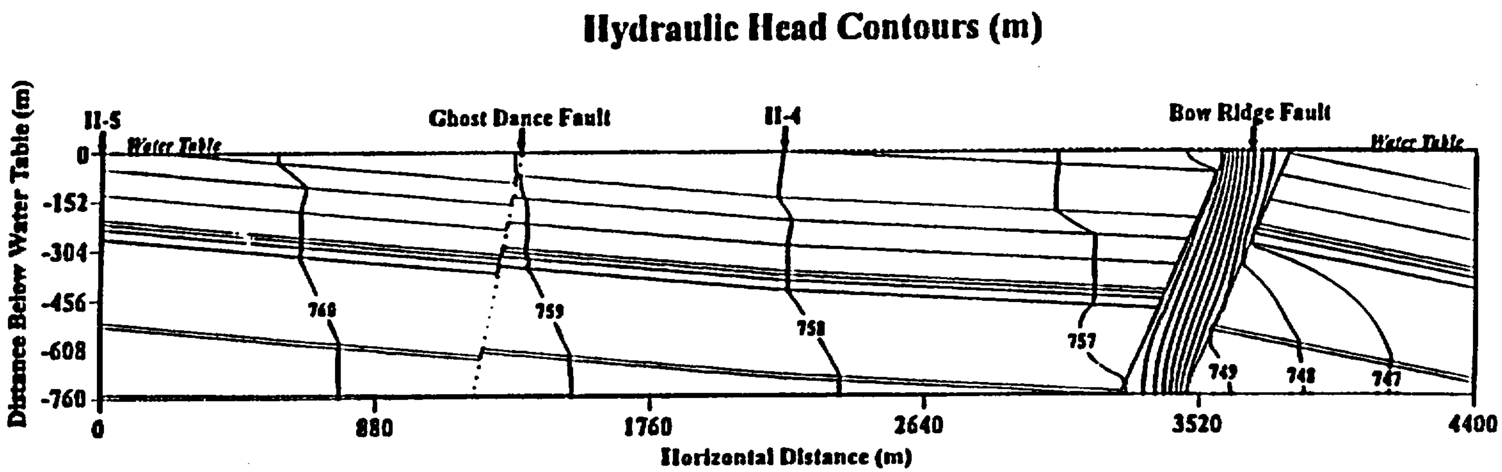
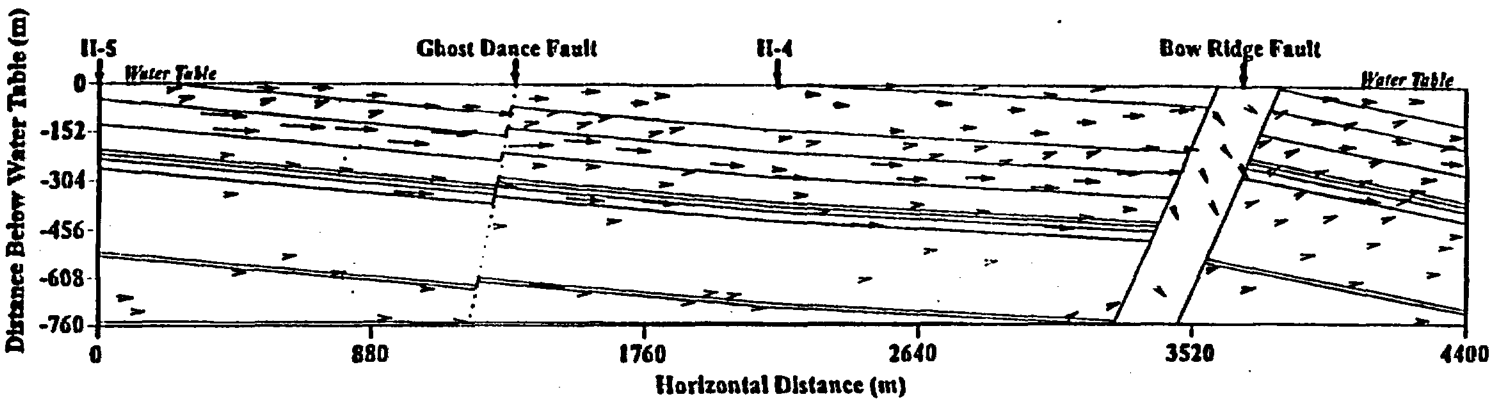


Figure 2-7. Hydraulic head fields for vertical cross section model; stratigraphic nomenclature taken from Whitfield et al. (1985)

Darcy Flux Vectors



Darcy Fluxes (m/yr)

Material Type	Minimum	Maximum
Calico Hills (CH)	0.030	0.79
Prow Pass 1 (PP1)	0.015	1.3
Prow Pass 2 (PP2)	0.018	0.27
Bullfrog (BF)	0.087	1.5
Bullfrog/Tram (BF/TR)	0.066	0.38
Tram 1 (TR1)	0.28	1.2
Tram 2 (TR2)	0.029	0.23
Tram 3 (TR3)	0.045	2.2
Tram 4 (TR4)	0.011	0.32
Lithic Ridge 1 (LR1)	0.041	2.9
Lithic Ridge 2 (LR2)	0.027	0.83
Bow Ridge	0.018	0.50

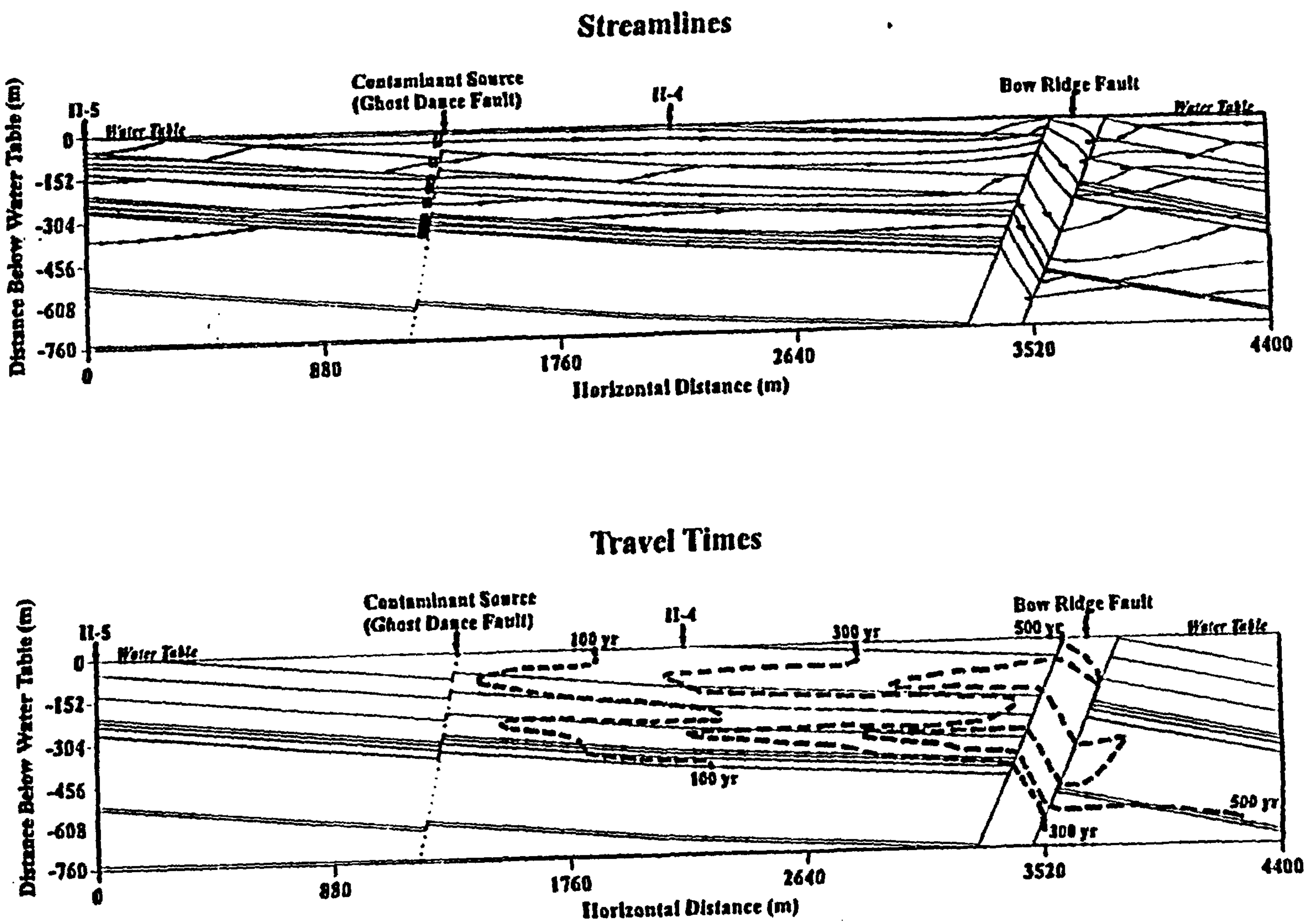


Figure 2-9. Pathlines and particle travel times for vertical cross-section flow model

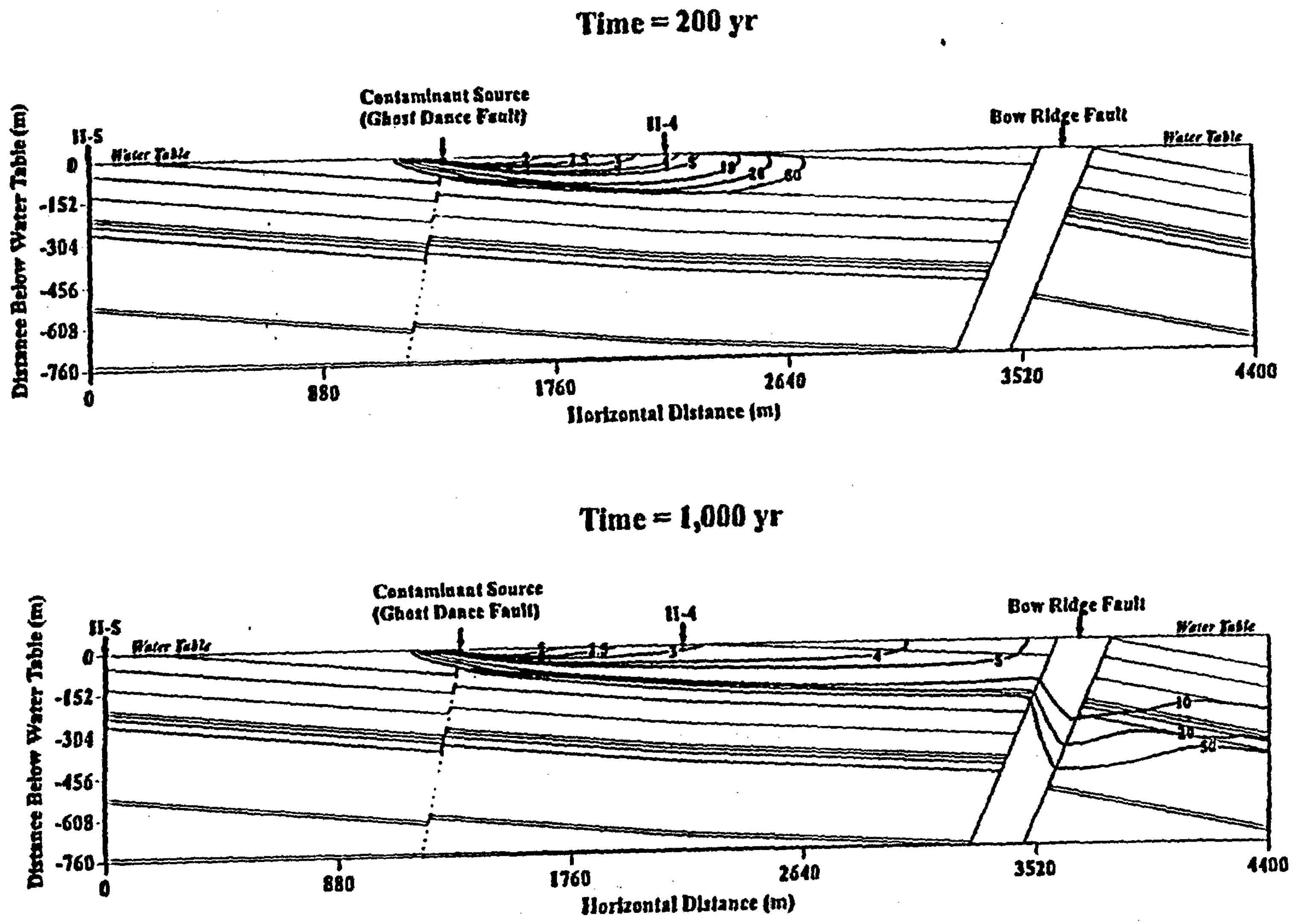
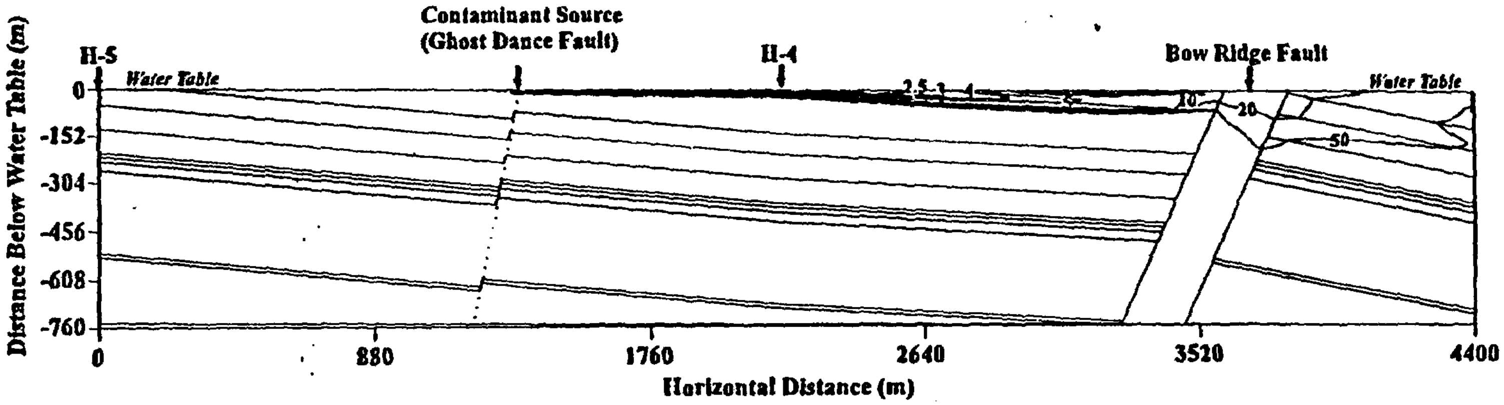
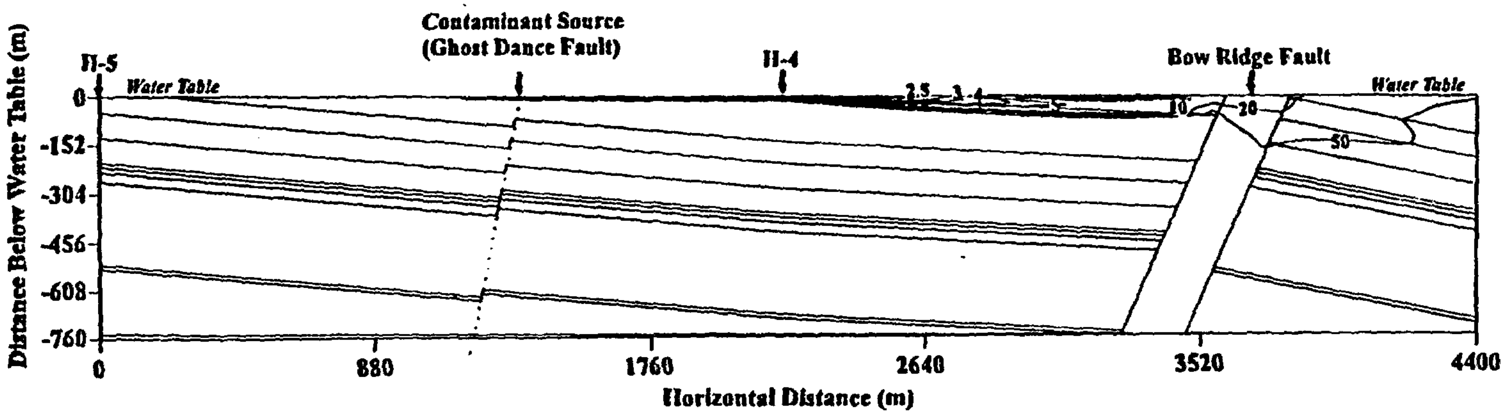


Figure 2-10. Radionuclide plume distributions for vertical cross section model with contour levels in terms of dilution factors

Time = 1,000 yr and Transverse Dispersivity = 0.03 m



Time = 1,000 yr and Transverse Dispersivity = 0.003 m



SUMMARY

Modeling Results

- Dilution factors (C_{max}/C) below the repository are low relative to TSPA-95 values
- Dipping layers can induce downward movement of plume
- Faults may have a important role in enhancing vertical plume spread

Future Work

- Application of three-dimensional models could provide better insights into mixing patterns and dilution magnitudes

ATTACHMENT 25

USE OF GROUNDWATER IN THE ARID AND SEMI-ARID WESTERN UNITED STATES: IMPLICATIONS FOR YUCCA MOUNTAIN AREA

Gordon W. Wittmeyer, Michael P. Miklas, and Richard V. Klar (CNWRA)
Derrik Williams and Donna Balin (Consultants)
Center for Nuclear Waste Regulatory Analyses
210/522-5082 gwitt@swri.org

November 5–6, 1997
DOE/NRC Technical Exchange on
Total System Performance Assessment for Yucca Mountain

PURPOSE AND SCOPE OF INVESTIGATION

- NAS recommendations may require determining the peak dose to the average member of a critical group, whose actual size, demographic makeup and lifestyle are in part defined as follows.

  > In the present and near future, these persons [the critical group] are real; that is, they are the persons now living in the near vicinity of the repository and in the direction of the postulated flow of the plume of radionuclides...The ICRP recommends use of present knowledge and cautious, but reasonable assumptions. (National Research Council, 1995)

- Withdrawal of land for NTS and Nellis AFB bombing range by the Federal Government has precluded private development in the immediate Yucca Mountain area.

- Need to examine the range of land and water use practices that may have occurred in the Yucca Mountain area before finalizing a description of the present critical group.

PURPOSE AND SCOPE OF INVESTIGATION (Cont'd)

- It may be reasonable to extrapolate water and land use practices from similar arid to semi-arid regions of the western U.S. to the Yucca Mountain region.

- A survey of well construction and water use practices in Arizona, southern Nevada, New Mexico, and the Trans-Pecos region of Texas was conducted to determine the likelihood that wells might have been drilled near Yucca Mountain where depths to water range from 300 to 700 m.

- Only climate and depth to groundwater were considered. Other factors such as water quality, proximity to railways and highways, occurrence of economic mineral deposits, and suitability of soils and topography for irrigated agriculture were not directly considered.

EXPLOITATION OF DEEP GROUNDWATER

- All other physiographic, climatologic, and socioeconomic factors being equal, water wells are drilled where the depth to water is small in order to limit development and production costs.

- Production costs are proportional to the product of pump discharge and lift.

  - Case 1. Domestic Well: 617 m^3 annual pumpage (around 150 gpd per person for a household of 3 persons), pumping from a depth of 30 m (approximately 100 ft). Annual production cost = Volume Pumped (617 m^3) × Pump Lift (30 m) × Unit Weight of Water (9,800 N/m^3) ÷ Efficiency (0.60) ÷ Conversion from Joules to Kilowatthours (3.6×10^6 J/kWh) × Unit Cost of Electricity (0.10 Dollars/kWh) = $8.40

  - Case 2. Irrigation Well: 1.52 m (5 ft) of water applied to 64.7 ha (160 acres) of cropland during the growing season pumped from a depth of 30 m (100 ft). Annual production cost = $13,386.

EXPLOITATION OF DEEP GROUNDWATER (Cont'd)

- If the pump lift for both the domestic and agricultural well is increased to 240 m (787 ft), annual energy costs rise to $67.20 and $107,085, respectively.

- Although both domestic and agricultural users would face the same percentage increase in variable pumping costs, one would expect the demand for domestic water to be much less price elastic than the demand for irrigation water.

- All other factors being equal, one would expect domestic use to predominate where depths to water are great and agricultural use to predominate where depths to water are small.

RESULTS OF WATER WELL SURVEY

Use of Water in Wells with Depths to Water Greater than 240 m in Arizona, southern Nevada, New Mexico, and the Trans-Pecos region of Texas.

State	Irrigation	Public	Stock	Industrial	Domestic	Commercial	Total with Specified Use
Arizona	2	33	12	3	13	0	63
Nevada	0	0	4	0	1	0	5
New Mexico	0	5	7	4	2	2	20
Trans-Pecos Texas	0	3	15	3	6	0	27
Totals (% Total)	2 (1.7)	41 (35.7)	38 (33.0)	10 (8.7)	22 (19.1)	2 (1.7)	115

INFERENCES FROM WATER WELL SURVEY

- Data generally support the hypothesis that irrigated agriculture is not commonly practiced where depths to water are great.

- Public water supply and stock water are the predominant uses where depths to water are great.

- Due to the large capital cost of installing a deep well, domestic use is less common than public or stock use.

- Capital costs of four archetypal wells for the Jackass Flat and Amargosa Desert region:

  - Well 1: (J-13 type well) Supplies 3000 people at 150 gpd per capita. Borehole depth 3,500 ft, Well depth 3,385 ft., Borehole diameter 26 in., Casing diameter 14 in., Screen length 2,162 ft, 700 gpm submersible @ static head of 1,000 ft. Capital cost $1,117,760. Total unit cost $1.20 per 1,000 gal.

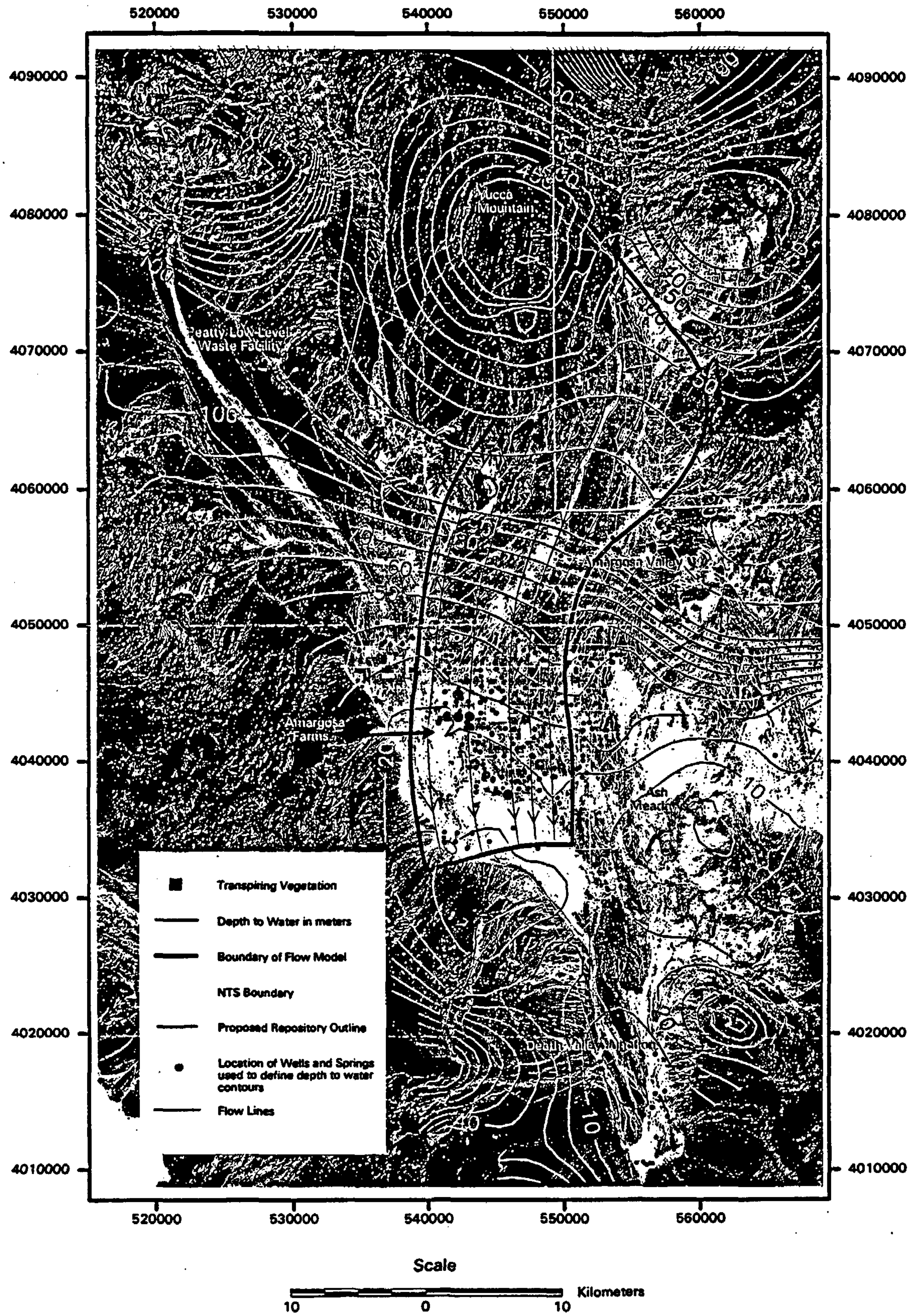
INFERENCES FROM WATER WELL SURVEY (Cont'd)

- Well 2: (J-12 type well) Supplies 3000 people at 150 gpd per capita. Borehole depth 900 ft., Well depth 887 ft., Borehole diameter 22 in., Casing diameter 12¾ in., Screen length 75 ft., 800 gpm submersible @ static head of 800 ft. Capital cost $229,145. Total unit cost $0.54 per 1,000 gal.

- Well 3: (Amargosa irrigation well) Supplies 5 ft. per season for a quarter-section center-pivot. Borehole depth 320 ft., Well depth 320 ft., Borehole diameter 28 in., Casing diameter 16 in., Screen length 150 ft., 2,400 gpm turbine shaft @ static head of 150 ft. Capital cost $167,745. Total unit cost $45 per acre-ft ($0.17 per 1,000 gal).

- Well 4: (Amargosa Valley public supply well) Supplies 40 people at 150 gpd per capita. Borehole depth 600 ft., Well depth 600 ft., Borehole diameter 19 in., Casing diameter 8 in., Screen length 200 ft., 10 gpm submersible @ static head of 300 ft. Capital cost $161,470. Total unit cost $7.91 per 1,000 gal.

Vegetation Map and Depth to Water: Yucca Mountain Region



INFERENCES FROM WATER WELL SURVEY (Cont'd)

- Data suggest that water use practices in the immediate Yucca Mountain area may have included a small cluster of homes supplied by one or more small-diameter, low-discharge, high-lift wells or a community or suburb supplied by wells similar in construction to J-13 or J-12.

- It is unlikely that irrigated agriculture would have occurred in the immediate Yucca Mountain vicinity due to the high unit cost of water.

ATTACHMENT 26

DOSE CONVERSION FACTORS FOR TPA VERSION 3.1 CODE

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NRC/DOE Technical Exchange on
Total System Performance Assessments for Yucca Mountain

DOSE CONVERSION FACTORS FOR TPA VERSION 3.1

- Background
- Objectives
- What are Dose Conversion Factors?
- Parameter Selections for DCF Calculations
  - Site-Specific Information
  - Generic Information
  - Identifying Parameters for Pluvial Conditions
- Summary

BACKGROUND

- IPA Phase 2 Used a Deterministic Population Dose Calculation Based on a Family Farming Scenario
- Initial CNWRA Study, Completed 10/95, Documented Site-Specific Information, and Included a Stochastic Individual Dose Calculation With Sensitivity Analysis
- NAS Recommended "The Use of a Standard That Sets a Limit on the Risk to Individuals" and that the "Critical Group Approach be Used in Yucca Mountain Standards"
- Initial CNWRA Study Updated (9/97) to Provide Basis for Dose Conversion Factors (DCFs) Used in TPA Version 3.1

OBJECTIVE

- Provide Capability in TPA Code to Convert Estimated Concentrations of Radionuclides in Groundwater and Surface Soil to Annual Total Effective Dose Equivalents (TEDEs).

  — Use Site-Specific Information to Define Receptor and Biosphere Parameters

  — Provide DCFs for All 43 (TSPA-93) Radionuclides

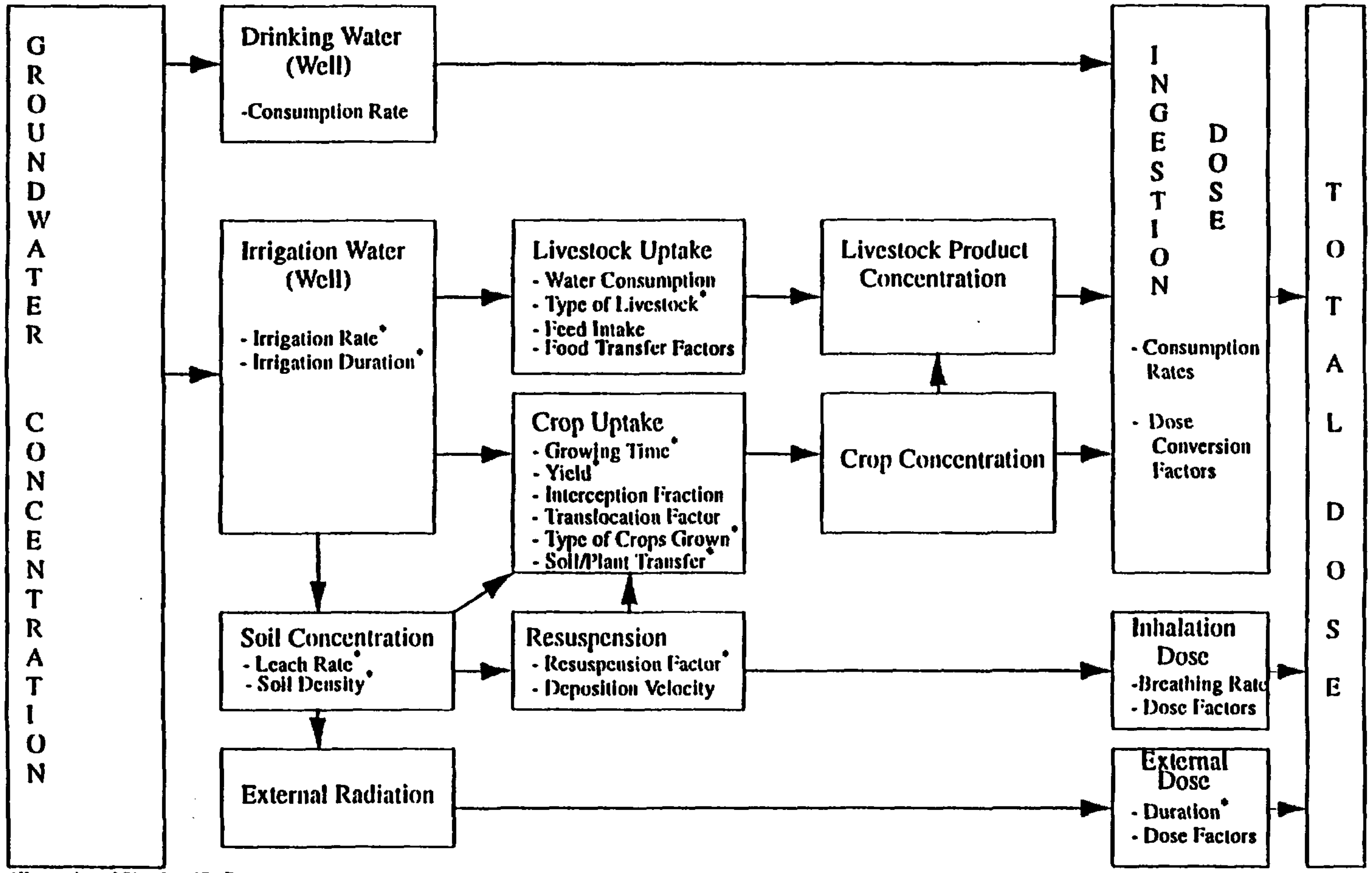
  — Include Consideration of Current and Pluvial Period Climate Conditions

  — Provide DCFs for Direct Releases

  — Use Sensitivity Analysis Results to Focus Parameter Selections

WHAT ARE DOSE CONVERSION FACTORS?

- As Used in TPA, a DCF is a Single Factor That Converts Concentration of Each Radionuclide in Soil or Water into a TEDE
  - Incorporates All Applicable Exposure Pathways and Exposure Scenario Assumptions
  - Surrogate for Dose Code Runs in TPA
  - One DCF Per Radionuclide, Exposure Pathway, Climate, and Contamination Source
  - DCFs Do Not Propagate Parameter Variation/Uncertainty, but Such Uncertainties Were Assessed Outside of TPA code



*Examples of Site Specific Parameters

PARAMETER SELECTIONS FOR DCFs

- For TPA Version 3.1 DCFs, the Average Member of the Most Highly Exposed Receptor Group was Approximated

  - Receptor Group Expected to Include the Highest Exposures
  - Average Member Estimated By Parameter Selections

- Sensitivity Analysis Results Focussed Attention on Parameters for Crop Interception, Resuspension, Food and Water Consumption Rates, Plant and Animal Uptake, and Irrigation Duration

- Current Exposure Scenario Conditions Were Assumed to be Constant Over Long Time Periods, Except When Major Climate Change is Expected (i.e., pluvial conditions)

- The High Likelihood of a Glacial Period in the Next 10k to 1000k Years Led to Consideration of Cooler and Wetter (i.e., Pluvial) Climate Conditions

PARAMETER SELECTIONS FOR DCFs

Examples of Site-Specific Information Used:

- Agricultural Water Use from Amargosa Permitted Withdrawals
- Local Insight from Amargosa Resident and Staff Visits to the Area
- Crop Interception Fractions from NTS and Other Research on Site-Relevant Crops (i.e., Alfalfa, Grasses)
- Soil Characterization Data for Farming Areas of Amargosa Valley
- Updated Leach Factors for Local Conditions (e.g., Sandy Soil, Irrigation Rate, Rainfall, Evapotranspiration)
- Local Recommendations for Desert Gardening: Crop Types and Growing Periods

PARAMETER SELECTIONS FOR DCFs

Examples of Generic Information Used:

- Plant and Animal Uptake Factors from IAEA
- Indoor/Outdoor Activity Times for Residents from NUREG/CR-5512 (i.e., Information for NRC Decommissioning Dose Calculations)
- Resuspension and Mass Loading Factors from IAEA and NUREG/CR-5512
- Food and Water Consumption Rates from NUREG/CR-5512, NRC Policy Guidance for Decommissioning No. 8-08, and EPA Exposure Factors Handbook.

PARAMETER SELECTIONS FOR DCFs

- Estimation of Parameters for Pluvial Conditions

  - Selected Pluvial Climate Analog Locations Based On:

    - MAP and MAT similar to estimates from paleoclimate record for YM pluvial (2x rainfall increase, 5 to 10 °C temperature decrease)

    - Terrestrial vegetation similar to SW Nevada during last glacial period

  - Agricultural and Soil Information for Blackfoot, ID Was Used to Estimate Pluvial Parameters for an Exposure Scenario. Crops Were Found to be Similar to Southern Nevada

  - Current Climate Parameters Affected by Rainfall and Temperature Changes Were Determined Directly or by Scaling Based Upon Differences Between Current Amargosa Climate Information and Pluvial Analog Site Data

PARAMETER SELECTIONS FOR DCFs

- Estimation of Parameters for Pluvial Conditions (cont'd)
  - No Attempt To Predict Future Human Practices — Focussed on What Might Exist Today Under Anticipated Pluvial Conditions
  - Effects of Predicted Increases in Surface Water and Potential Impacts on Human Practices and Surface Transport of Contamination Were Not Considered
- Results
  - Pluvial DCFs Are Approximately 60 to 70 Percent of DCFs for the Current Climate. This Corresponds to the Reduction in Irrigation Water Use in Under Predicted Pluvial Conditions.

SUMMARY

- NRC/CNWRA Has Provided the Capability in TPA Version 3.1 to Convert Soil and Groundwater Concentrations to Doses for Current and Pluvial Period Climate Conditions
- DCFs Were Determined for Each Radionuclide, Transport Pathway (groundwater and air), Exposure Pathway, Climate, and Receptor Type.
- DCFs Are Based Upon Site–Specific and Generic Information and Can Be Updated, As Needed, When New Information Becomes Available
- Sensitivity Analysis Results Were Used to Focus DCF Parameter Selections
- Additional Documentation is Provided in CNWRA Report 97-009

ATTACHMENT 27

BIOMASS SUMMARY

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BIOMASS

- INTERNATIONAL ATOMIC ENERGY AGENCY PROGRAM
- BIOSPHERE MODELING AND ASSESSMENT METHODS
- DEVELOPED OUT OF BOTH BIOMOVS II AND IAEA'S VALIDATION OF ENVIRONMENTAL MODEL PREDICTIONS (VAMP) PROGRAMS
- THREE AREAS OF FOCUS
  - THEME 1: RADIOACTIVE WASTE DISPOSAL
    - IMPLEMENTATION AND AUGMENTATION OF REFERENCE BIOSPHERE METHODOLOGY
  - THEME 2: ENVIRONMENTAL RELEASES
    - DOSE RECONSTRUCTION
    - ENVIRONMENTAL REMEDIATION
  - THEME 3: BIOSPHERIC PROCESSES
    - TRITIUM
    - FRUIT TREE

NRC INVOLVEMENT AND UTILIZATION

- OBSERVERS IN BIOMOVS II SINCE 1994
- PARTICIPANTS IN BIOMASS PROGRAM THEME 1
- USED REFERENCE BIOSPHERE AND CRITICAL GROUP APPROACH IN CALCULATIONS SUPPORTING DISCUSSIONS WITH EPA
- SUPPORT USE OF REFERENCE BIOSPHERE AND CRITICAL GROUP IN WASTE DISPOSAL AND DECOMMISSIONING
- CONSIDERING THE INTERNATIONAL APPROACH AND SELECTION CRITERIA FOR USE IN NRC ACTIVITIES